Applied Machine Learning

Supervised machine learning (Part 1)

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Learning objectives

- **Understand how a number of different supervised learning algorithms learn by estimating their parameters from data to make new predictions.**
- **Understand the strengths and weaknesses of particular supervised learning methods.**

Learning objectives

- **Learn how to apply specific supervised machine learning algorithms in Python with scikit-learn.**
- **Learn about general principles of supervised machine learning, like overfitting and how to avoid it.**

Review of important terms

- **Feature representation**
- **Data instances/samples/ examples (X)**
- **Target value (y)**

```
fruits
```

	fruit_label	fruit_name	fruit_subtype	mass	width	height	color_score
0	1	apple	granny_smith	192	8.4	7.3	0.55
1	1	apple	granny_smith	180	8.0	6.8	0.59
2	1	apple	granny_smith	176	7.4	7.2	0.60
3	2	mandarin	mandarin	86	6.2	4.7	0.80
4	2	mandarin	mandarin	84	6.0	4.6	0.79
5	2	mandarin	mandarin	80	5.8	4.3	0.77
6	2	mandarin	mandarin	80	5.9	4.3	0.81
7	2	mandarin	mandarin	76	5.8	4.0	0.81
8	1	apple	braeburn	178	7.1	7.8	0.92
9	1	apple	braeburn	172	7.4	7.0	0.89
10	1	apple	braeburn	166	6.9	7.3	0.93
11	1	apple	braeburn	172	7.1	7.6	0.92
12	1	apple	braeburn	154	7.0	7.1	0.88
13	1	apple	golden_delicious	164	7.3	7.7	0.70
14	1	apple	golden_delicious	152	7.6	7.3	0.69
15	1	apple	golden_delicious	156	7.7	7.1	0.69
16	1	apple	golden_delicious	156	7.6	7.5	0.67
17	1	apple	golden_delicious	168	7.5	7.6	0.73
18	1	apple	cripps_pink	162	7.5	7.1	0.83

Review of important terms

- **Training and test sets**
- **Model/Estimator**
  - *Model fitting produces a 'trained model'.*
  - *Training is the process of estimating model parameters.*
- **Evaluation method**

```
%matplotlib notebook
import numpy as np
import pandas as pd
import seaborn as sn
import matplotlib.pyplot as plt

from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier

fruits = pd.read_table('fruit_data_with_colors.txt')

X = fruits[['height', 'width', 'mass', 'color_score']]
y = fruits['fruit_label']

X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

knn = KNeighborsClassifier(n_neighbors = 5)
knn.fit(X_train, y_train)
print("Accuracy of K-NN classifier on test set: ", knn.score(X_test, y_test))

example_fruit = [[5.5, 2.2, 10, 0.70]]
print("Predicted fruit type for ", example_fruit, " is ", knn.predict(example_fruit))
```

Applied Machine Learning

Overfitting and Underfitting

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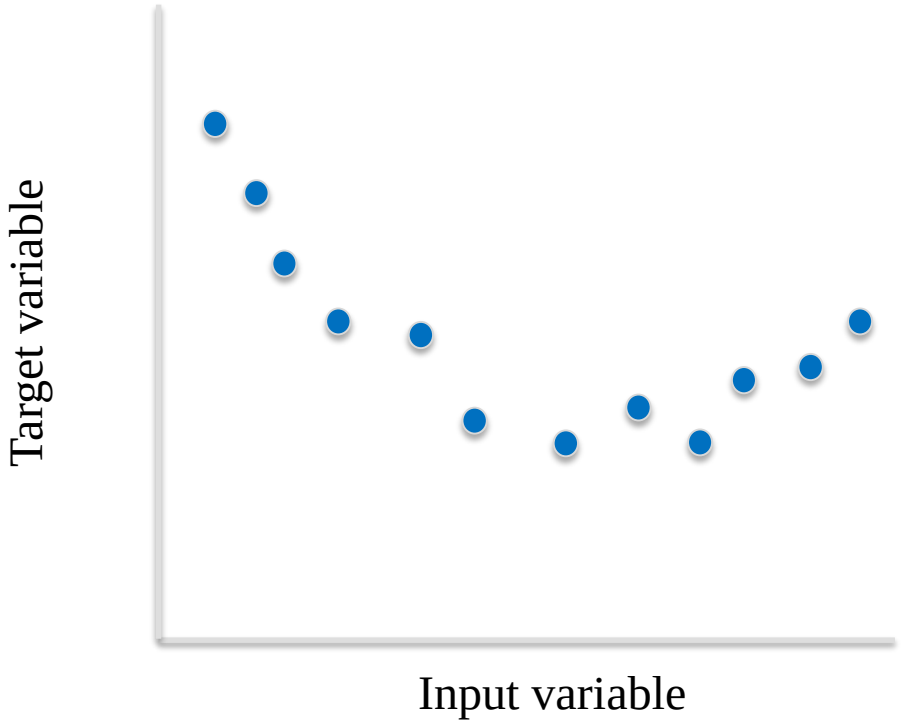
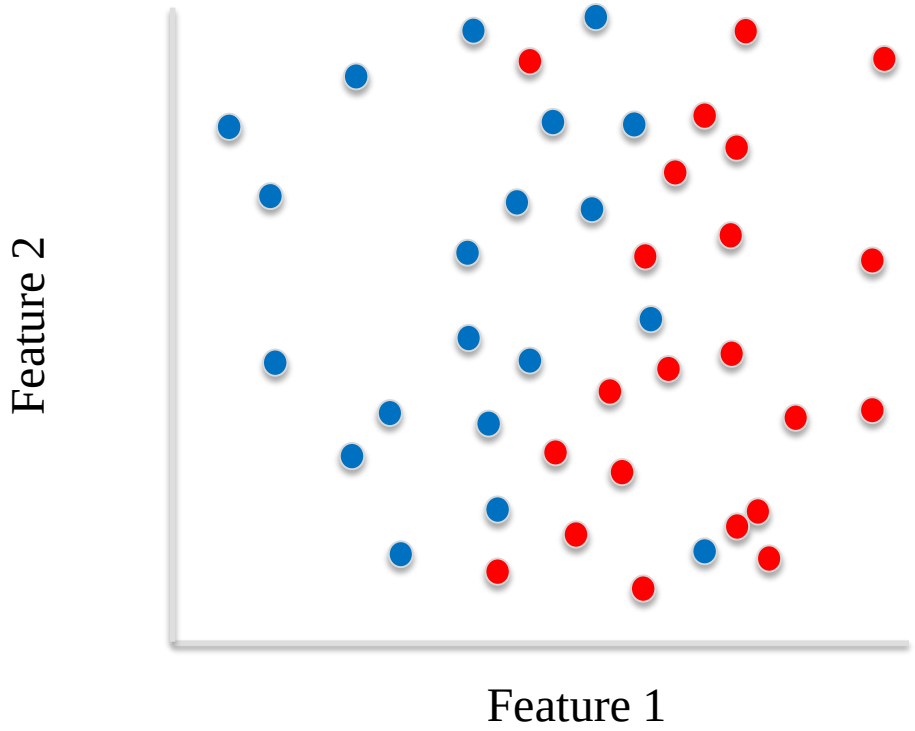
Generalization, Overfitting, and Underfitting

- **Generalization ability refers to an algorithm's ability to give accurate predictions for new, previously unseen data.**
- **Assumptions:**
  - *Future unseen data (test set) will have the same properties as the current training sets.*
  - *Thus, models that are accurate on the training set are expected to be accurate on the test set.*
  - *But that may not happen if the trained model is tuned too specifically to the training set.*
- **Models that are too complex for the amount of training data available are said to overfit and are not likely to generalize well to new examples.**
- **Models that are too simple, that don't even do well on the training data, are said to underfit and also not likely to generalize well.**

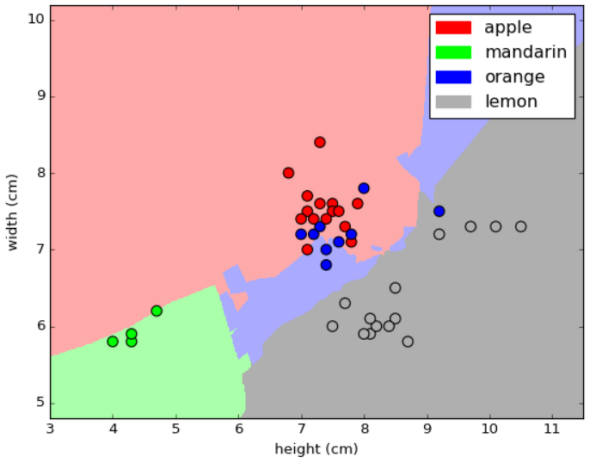
Overfitting in regression



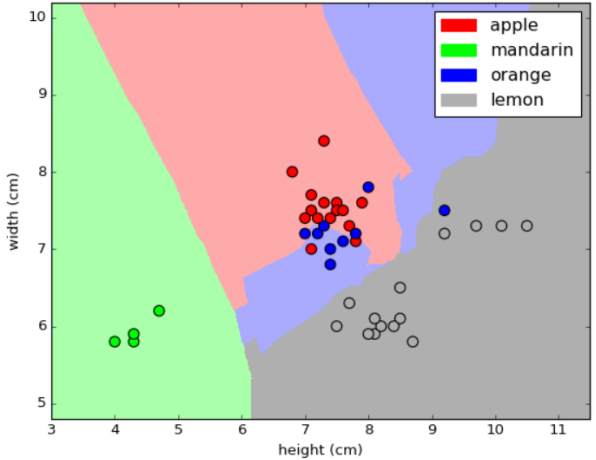
Overfitting in classification



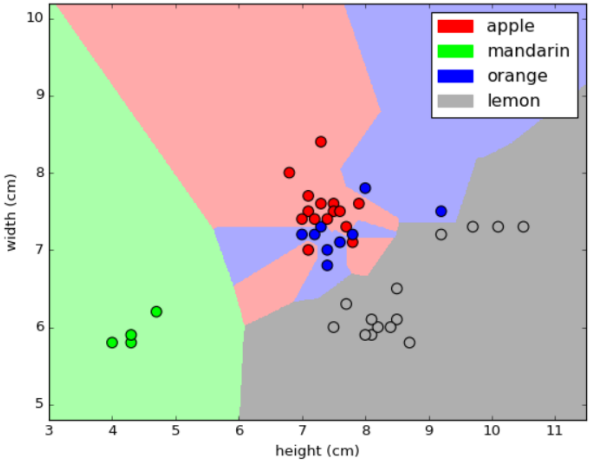
Overfitting with k-NN classifiers



K=10



K=5



K=1

Applied Machine Learning

Supervised learning: Datasets

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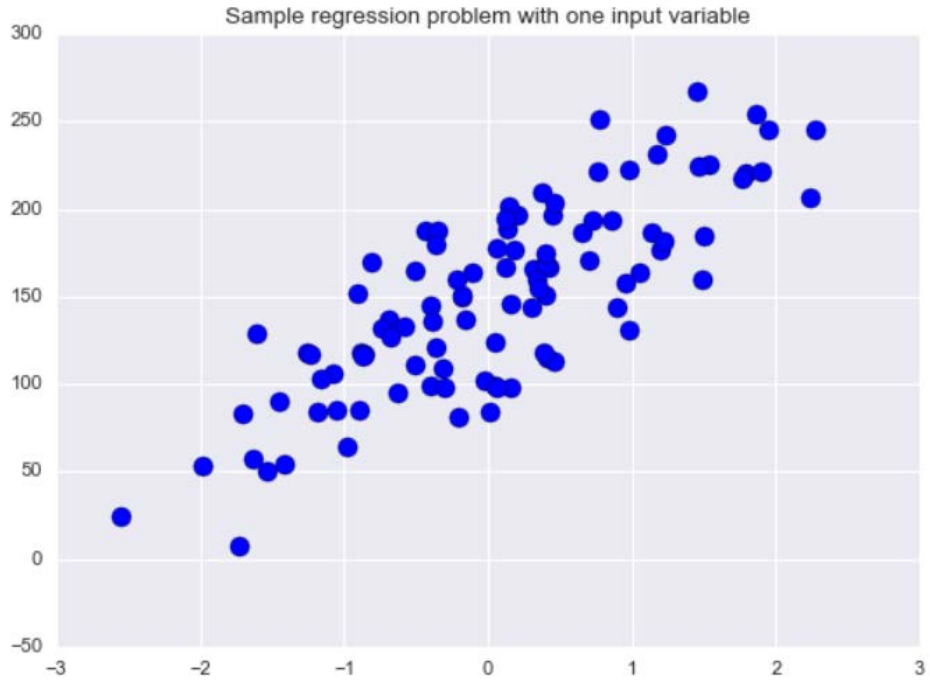
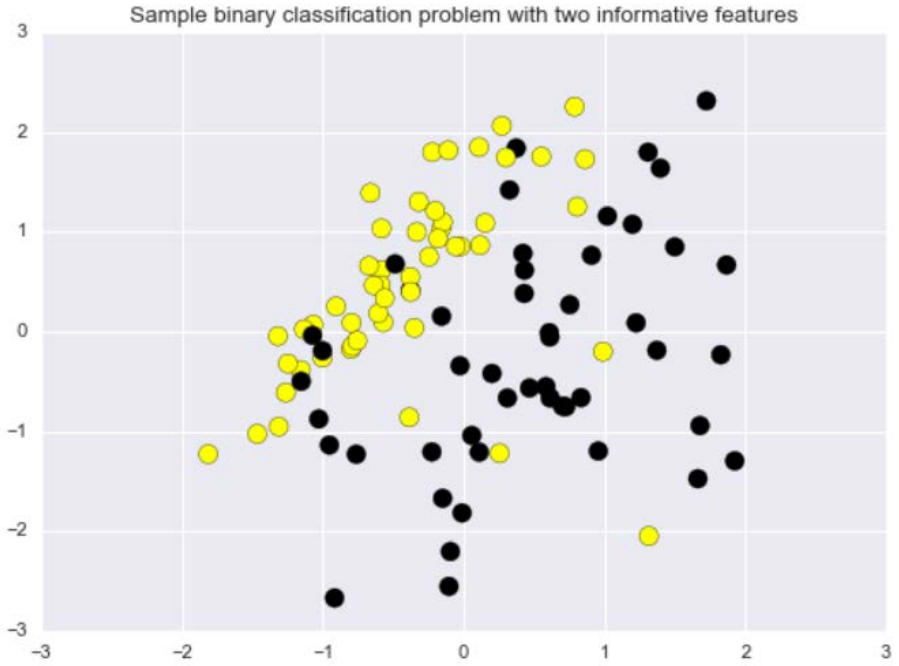
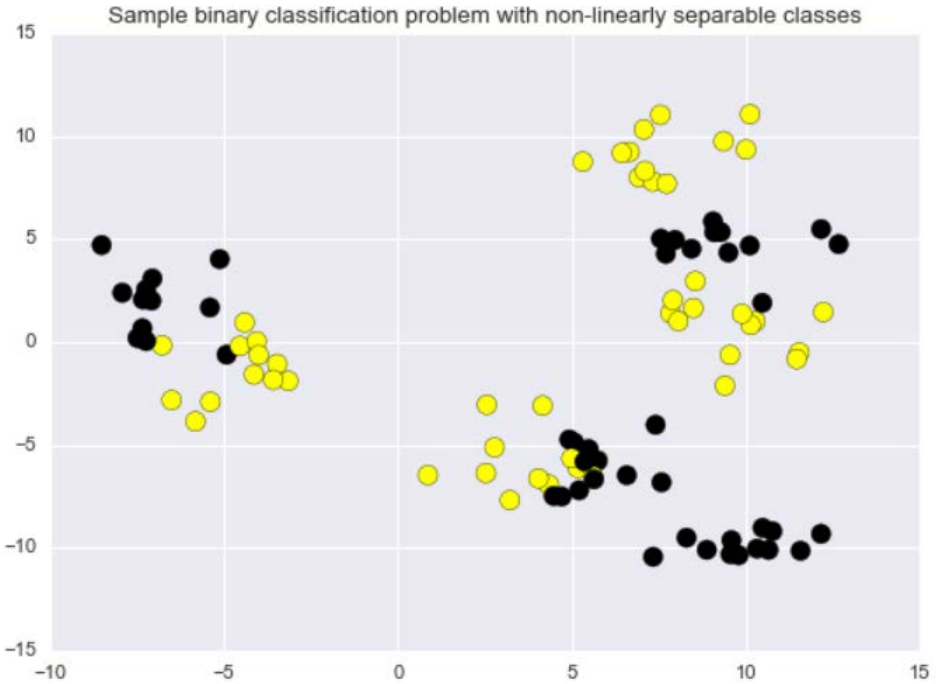
Simple Regression Dataset



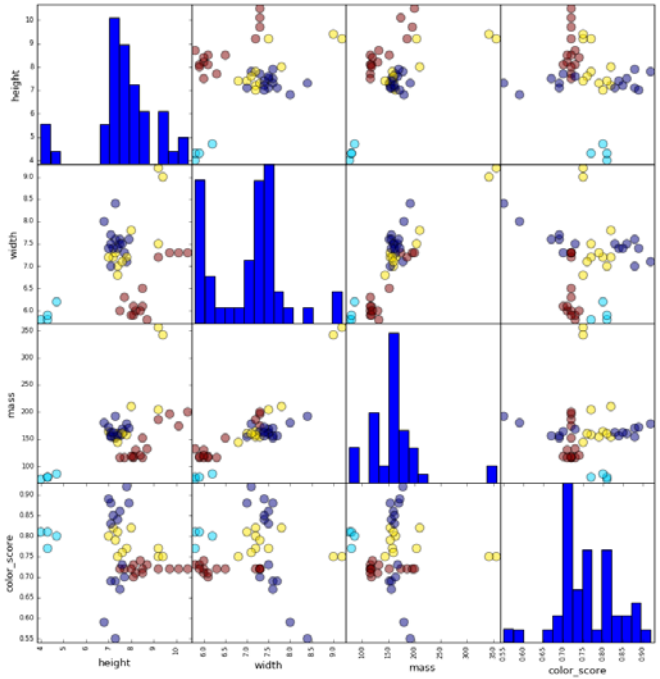
Simple Binary Classification Dataset



Complex Binary Classification Dataset



Fruits Multi-class Classification Dataset



Features

- **`width`**
- **`height`**
- **`mass`**
- **`color_index`**

Classes

0: apple

1: mandarin orange

2: orange

3: lemon

Communities and Crime Dataset

	population	householdsize	agePct12t21	agePct12t29	agePct16t24	agePct65up	numbUrban	pctUrban	medIncome	pctWWage	...	MedRentP
0	11980	3.10	12.47	21.44	10.93	11.33	11980	100.0	75122	89.24	...	23.8
1	23123	2.82	11.01	21.30	10.48	17.18	23123	100.0	47917	78.99	...	27.6
2	29344	2.43	11.36	25.88	11.01	10.28	29344	100.0	35669	82.00	...	24.1
3	16656	2.40	12.55	25.20	12.19	17.57	0	0.0	20580	68.15	...	28.7
5	140494	2.45	18.09	32.89	20.04	13.26	140494	100.0	21577	75.78	...	26.4
6	28700	2.60	11.17	27.41	12.76	14.42	28700	100.0	42805	79.47	...	24.4
7	59459	2.45	15.31	27.93	14.78	14.60	59449	100.0	23221	71.60	...	26.3
8	74111	2.46	16.64	35.16	20.33	8.58	74115	100.0	25326	83.69	...	25.2
9	103590	2.62	19.88	34.55	21.62	13.12	103590	100.0	17852	74.20	...	29.6
10	31601	2.54	15.73	28.57	15.16	14.26	31596	100.0	24763	73.92	...	23.8

Input features:
socio-economic data by location from U.S. Census

Target variable:
Per capita violent crimes

Derived from the original UCI dataset at:

https://archive.ics.uci.edu/ml/datasets/Communities+and+Crime+Unnormalized

```
from adspy_shared_utilities import load_crime_dataset
crime = load_crime_dataset()
```

Applied Machine Learning

K-Nearest Neighbors: Classification and Regression

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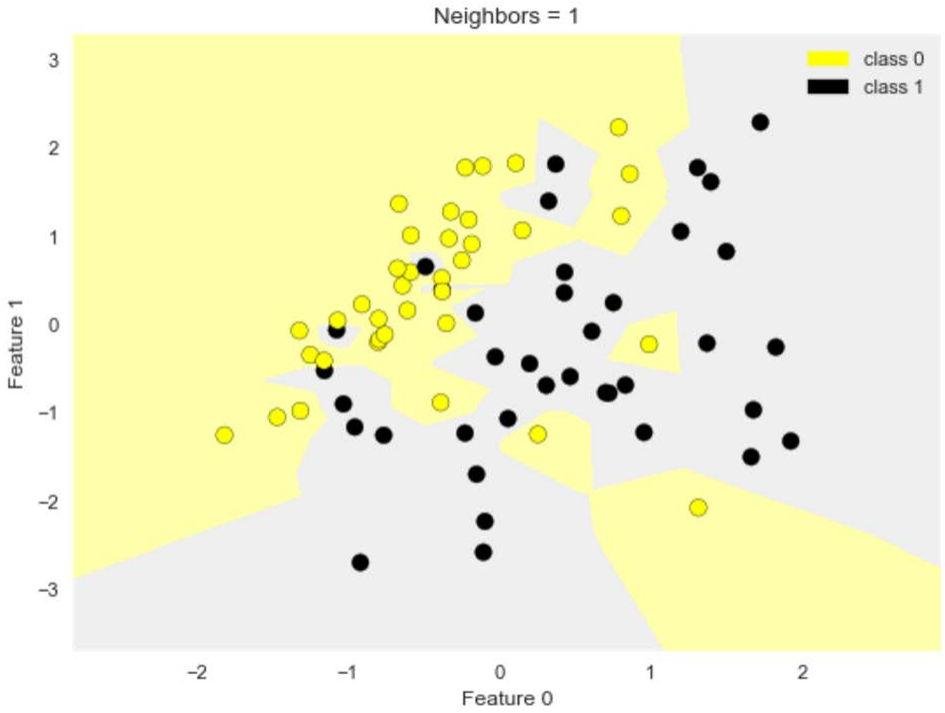
The k-Nearest Neighbor (k-NN) Classifier Algorithm

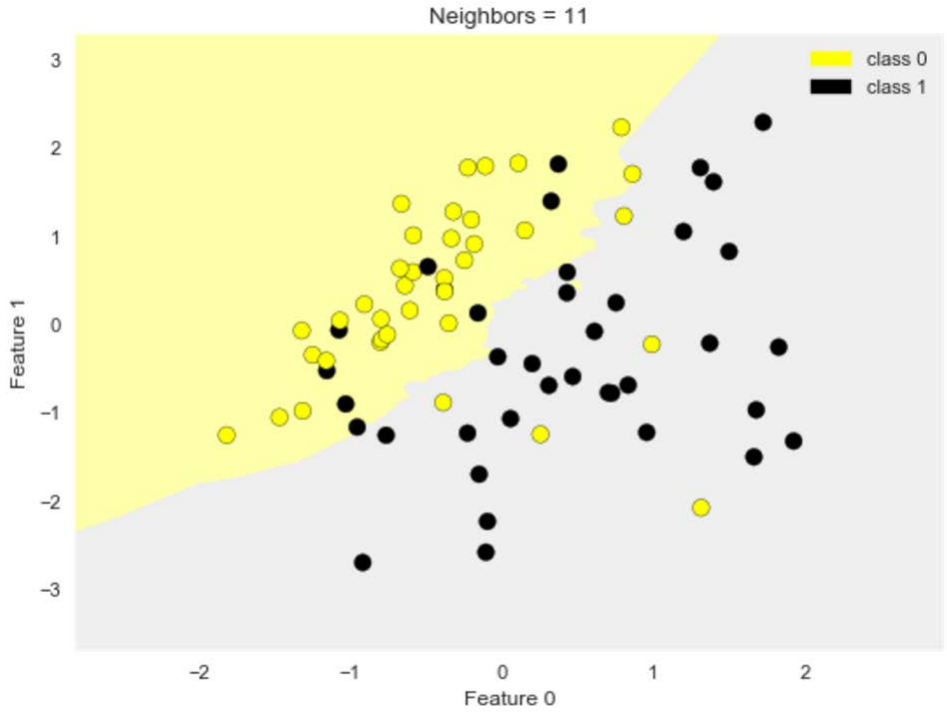
Given a training set X_train with labels y_train, and given a new instance x_test to be classified:

1. **Find the most similar instances (let's call them X_NN) to x_test that are in X_train.**
2. **Get the labels y_NN for the instances in X_NN**
3. **Predict the label for x_test by combining the labels y_NN**
   e.g. simple majority vote

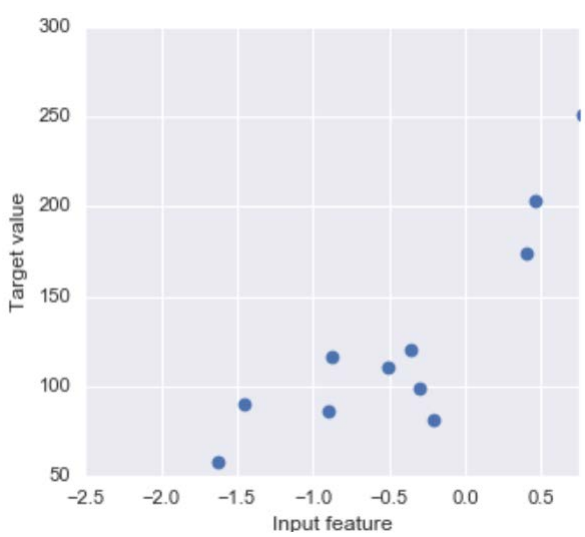
Nearest Neighbors Classification (k=1)

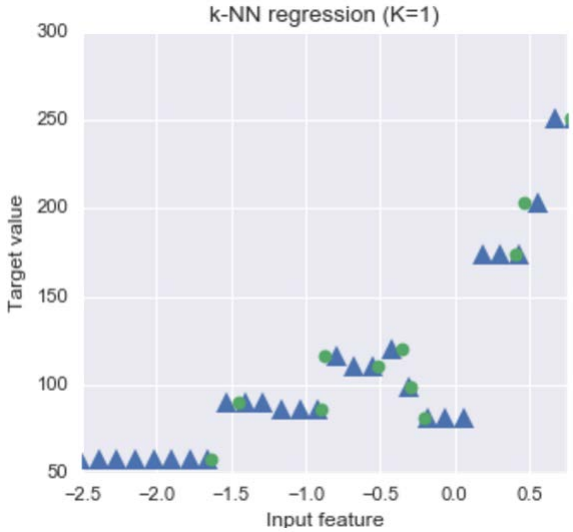


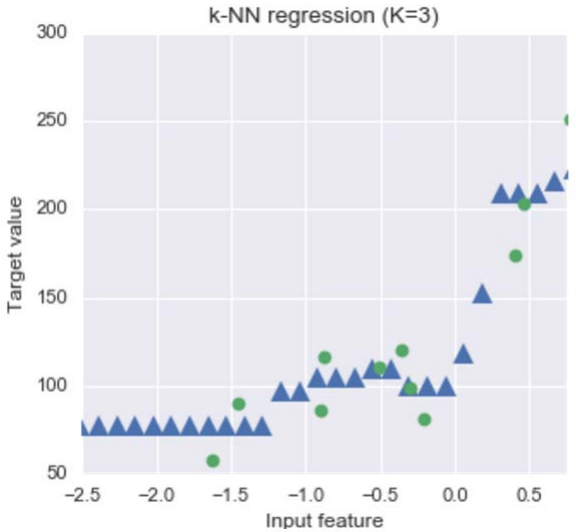
Nearest Neighbors Classification (k = 11)



k-Nearest Neighbors Regression







The R^2 ("r-squared") Regression Score

- **Measures how well a prediction model for regression fits the given data.**
- **The score is between 0 and 1:**
  - *A value of 0 corresponds to a constant model that predicts the mean value of all training target values.*
  - *A value of 1 corresponds to perfect prediction*
- **Also known as "coefficient of determination"**

KNeighborsClassifier and KNeighborsRegressor: important parameters

Model complexity

- ***n_neighbors :*** **number of nearest neighbors (k) to consider**
  - *Default = 5*

Model fitting

- ***metric: distance function between data points***
  - *Default: Minkowski distance with power parameter p = 2 (Euclidean)*

Applied Machine Learning

Linear Regression: Least-Squares

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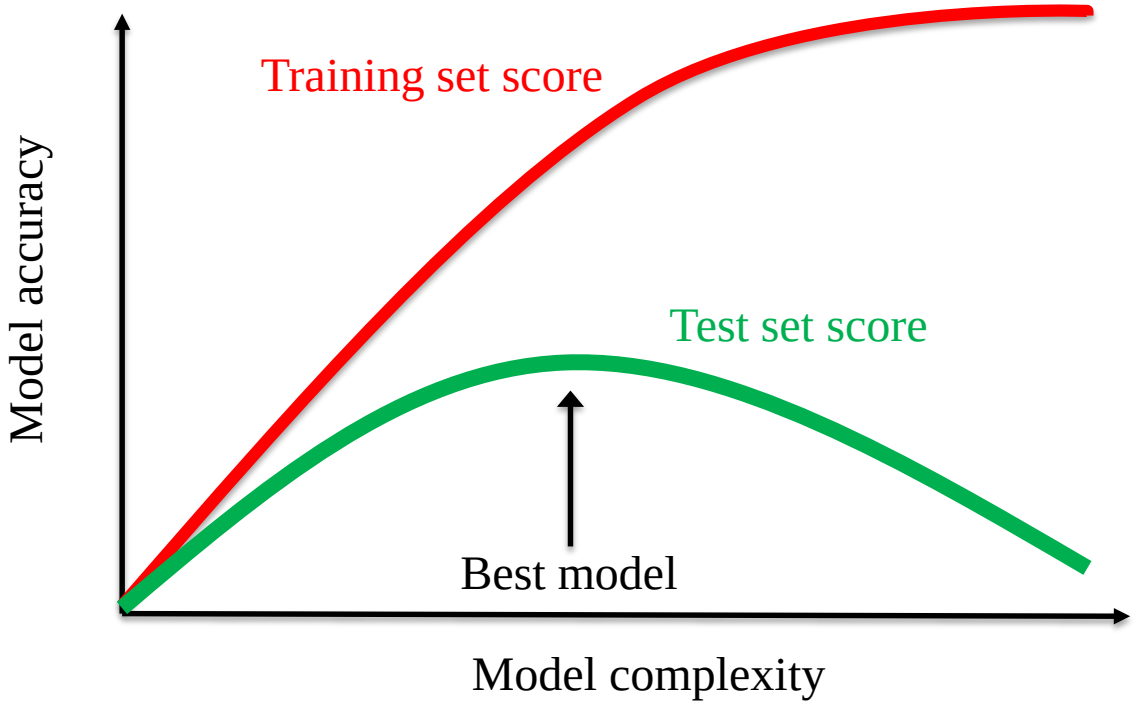
Supervised learning methods: Overview

- **To start with, we'll look at two simple but powerful prediction algorithms:**
  - *K-nearest neighbors (review from week 1, plus regression)*
  - *Linear model fit using least-squares*
- **These represent two complementary approaches to supervised learning:**
  - *K-nearest neighbors makes few assumptions about the structure of the data and gives potentially accurate but sometimes unstable predictions (sensitive to small changes in the training data).*
  - *Linear models make strong assumptions about the structure of the data and give stable but potentially inaccurate predictions.*

Supervised Learning Methods: Overview

- **We'll cover a number of widely-used supervised learning methods for classification and regression.**
- **For each supervised learning method we'll explore:**
  - *How the method works conceptually at a high level.*
  - *What kind of feature preprocessing is typically needed.*
  - *Key parameters that control model complexity, to avoid under- and over-fitting.*
  - *Positives and negatives of the learning method.*

The relationship between model complexity and training/test performance



Linear Models

- **A linear model is a <u>sum of weighted variables</u> that predicts a target output value given an input data instance. <u>Example</u>: *predicting housing prices***
  - *House features: taxes per year (X_{TAX}), age in years (X_{AGE})*

$$\widehat{Y_{PRICE}} = 212000 + 109\, X_{TAX} - 2000\, X_{AGE}$$

  - *A house with feature values (X_{TAX}, X_{AGE}) of (10000, 75) would have a predicted selling price of:*

$$\widehat{Y_{PRICE}} = 212000 + 109 \cdot \mathbf{10000} - 2000 \cdot \mathbf{75} = \mathbf{1{,}152{,}000}$$

Linear Regression is an Example of a Linear Model

Input instance – feature vector: $\boldsymbol{x} = (x_0, x_1, \ldots, x_n)$

Predicted output:

$$\hat{y} = \widehat{w_0} x_0 + \widehat{w_1} x_1 + \cdots \widehat{w_n} x_n + \hat{b}$$

Parameters to estimate:

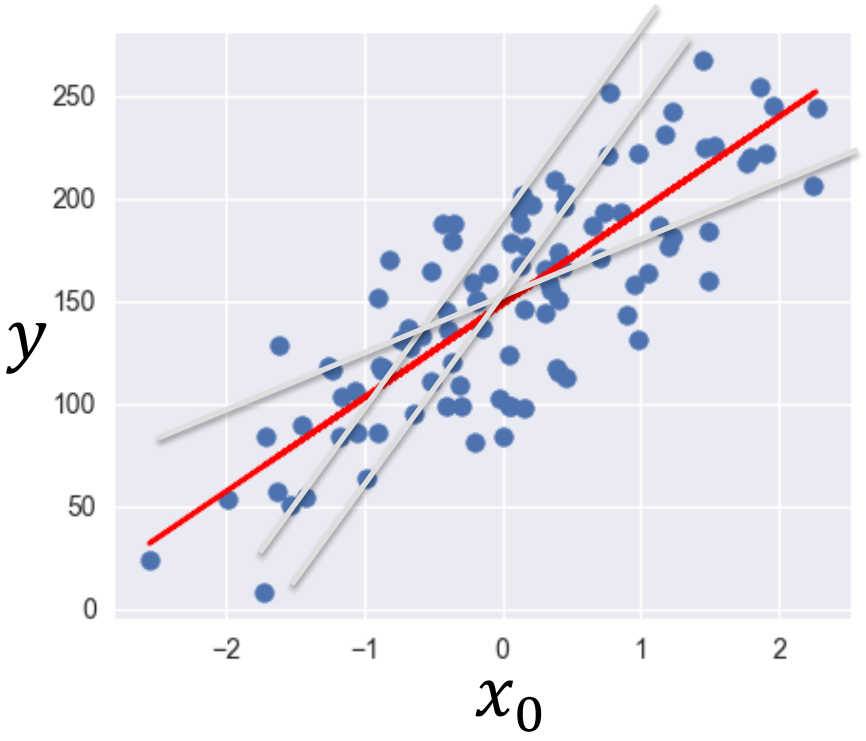
- $\widehat{\boldsymbol{w}} = (\widehat{w_0}, \cdots, \widehat{w_n})$: feature weights/ model coefficients
- $\widehat{\boldsymbol{b}}$: constant bias term / intercept

A Linear Regression Model with one Variable (Feature)

Input instance: $\boldsymbol{x} = (x_0)$

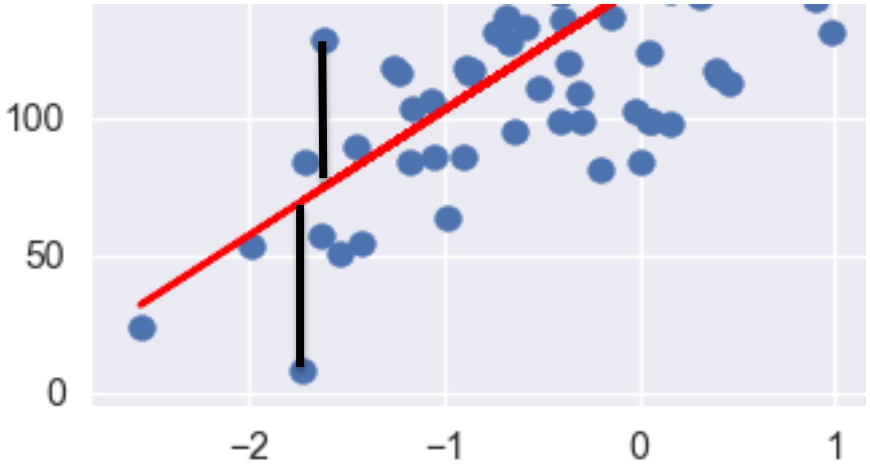
Predicted output: $\hat{y} = \widehat{w_0} x_0 + \hat{b}$

Parameters to estimate: $\widehat{w_0}$ (slope)
$\hat{b}$ (y-intercept)



Least-Squares Linear Regression ("Ordinary least-squares")

- Finds *w* and *b* that minimizes the mean squared error of the linear model: the sum of squared differences between predicted target and actual target values.
- No parameters to control model complexity.

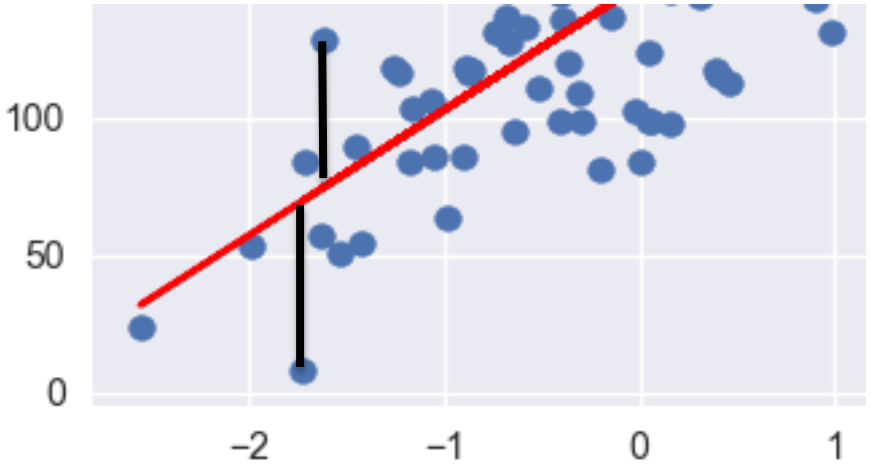


How are Linear Regression Parameters *w*, *b* Estimated?

- **Parameters are estimated from training data.**
- **There are many different ways to estimate *w* and *b*:**
  - *Different methods correspond to different "fit" criteria and goals and ways to control model complexity.*
- **The learning algorithm finds the parameters that optimize an objective function, typically to minimize some kind of loss function of the predicted target values *vs.* actual target values.**

Least-Squares Linear Regression ("Ordinary least-squares")

- Finds *w* and *b* that minimizes the sum of squared differences (RSS) over the training data between predicted target and actual target values.
- a.k.a. mean squared error of the linear model
- No parameters to control model complexity.



$$RSS(\boldsymbol{w}, b) = \sum_{\{i=1\}}^{N} (\boldsymbol{y}_i - (\boldsymbol{w} \cdot \boldsymbol{x}_i + b))^2$$

Least-Squares Linear Regression ("Ordinary Least-Squares")

- Finds *w* and *b* that minimizes the sum of squared differences (RSS) over the training data between predicted target and actual target values.
- a.k.a. mean squared error of the linear model
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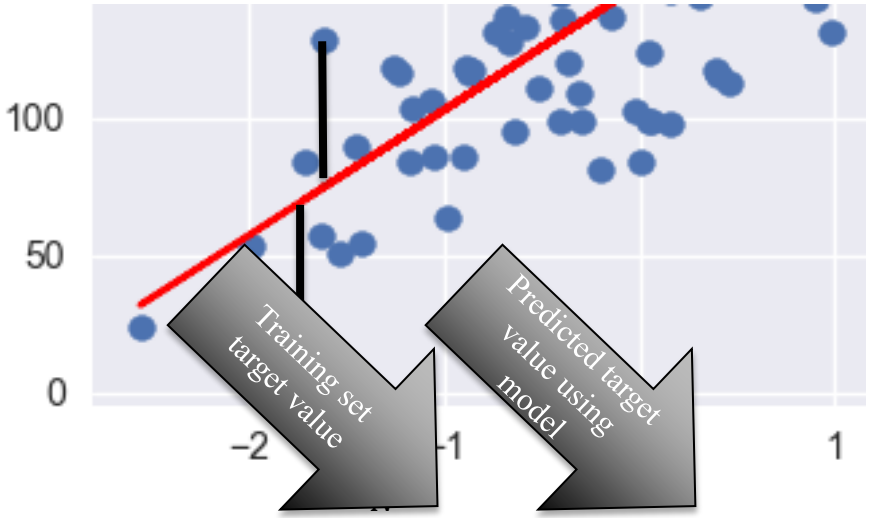


$$RSS(\boldsymbol{w}, b) = \sum_{\{i=1\}} (\boldsymbol{y}_i - (\boldsymbol{w} \cdot \boldsymbol{x}_i + b))^2$$

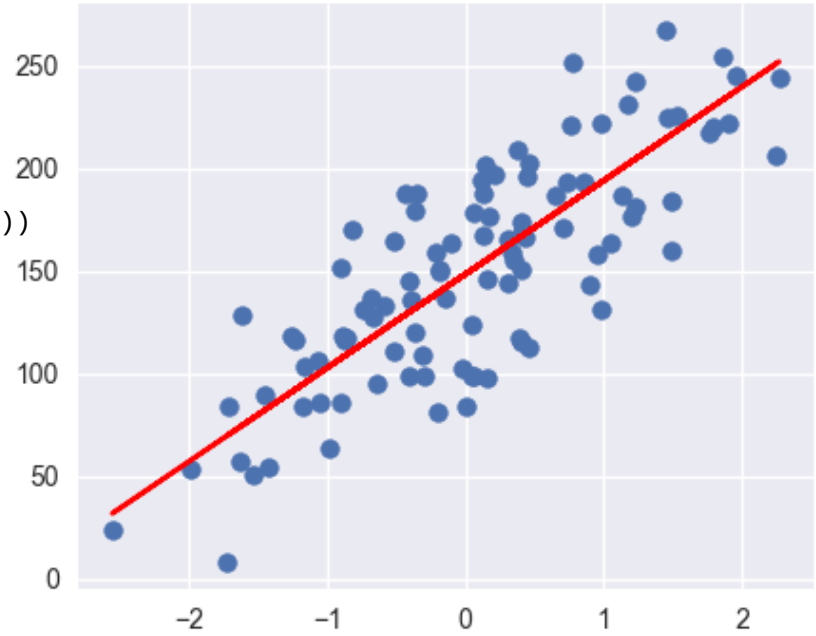
Least-Squares Linear Regression in Scikit-Learn

```
from sklearn.linear_model import LinearRegression

X_train, X_test, y_train, y_test =
      train_test_split(X_R1, y_R1, random_state = 0)

linreg = LinearRegression().fit(X_train, y_train)

print("linear model intercept (b): {}".format(linreg.intercept_))
print("linear model coeff (w): {}".format(linreg.coef_))
```



linreg.coef_ linreg.intercept_

$$\hat{y} = \boldsymbol{w_0} x_0 + b$$

Least-Squares Linear Regression in Scikit-Learn

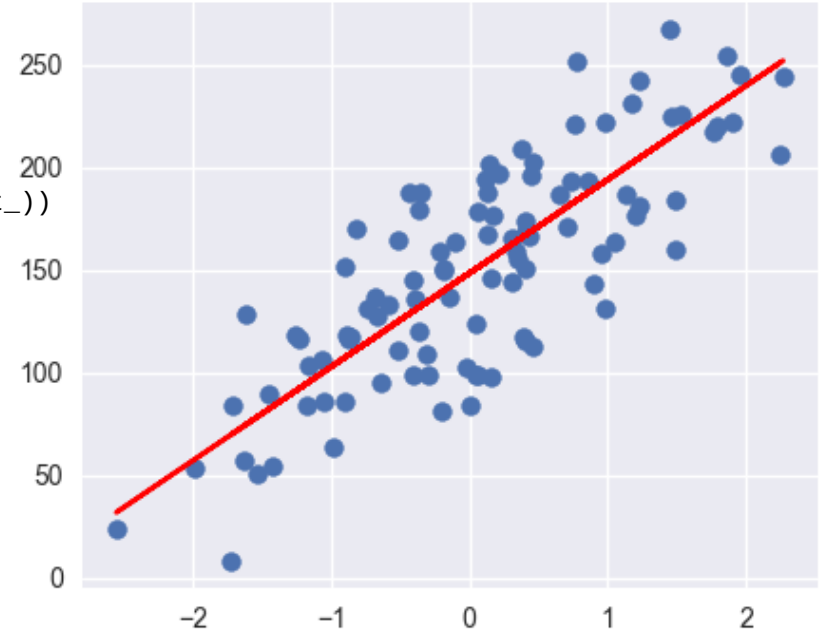
```
from sklearn.linear_model import LinearRegression

X_train, X_test, y_train, y_test =
      train_test_split(X_R1, y_R1, random_state = 0)

linreg = LinearRegression().fit(X_train, y_train)

print("linear model intercept (b): {}".format(linreg.intercept_))
print("linear model coeff (w): {}".format(linreg.coef_))
```

Underscore denotes a quantity derived from training data, as opposed to a user setting.



`linreg.coef_` `linreg.intercept_`

$$\hat{y} = \boldsymbol{w_0} x_0 + b$$

Least-Squares Linear Regression in Scikit-Learn

```
from sklearn.linear_model import LinearRegression

X_train, X_test, y_train, y_test =
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linreg = LinearRegression().fit(X_train, y_train)

print("linear model intercept (b): {}".format(linreg.intercept_))
print("linear model coeff (w): {}".format(linreg.coef_))
```
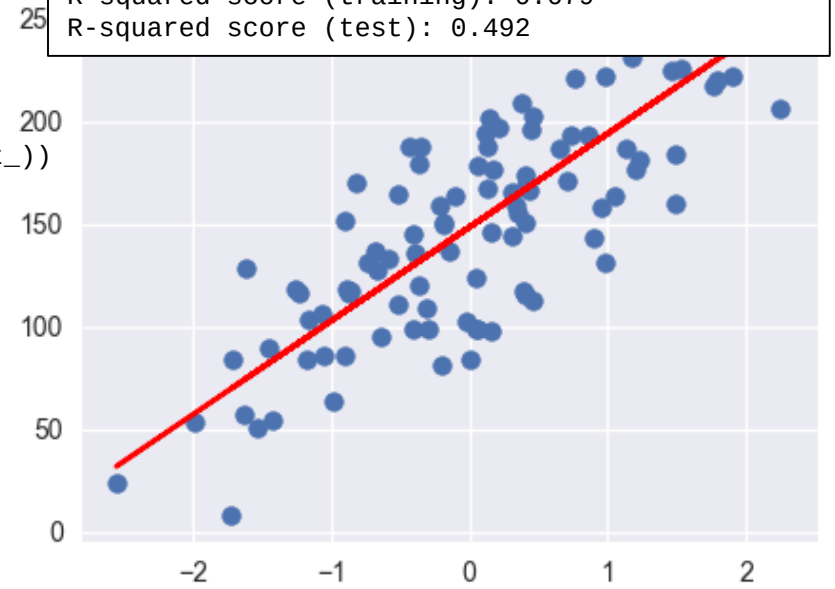

```
linear model coeff (w): [ 45.70870465]
linear model intercept (b): 148.44575345658873
R-squared score (training): 0.679
R-squared score (test): 0.492
```



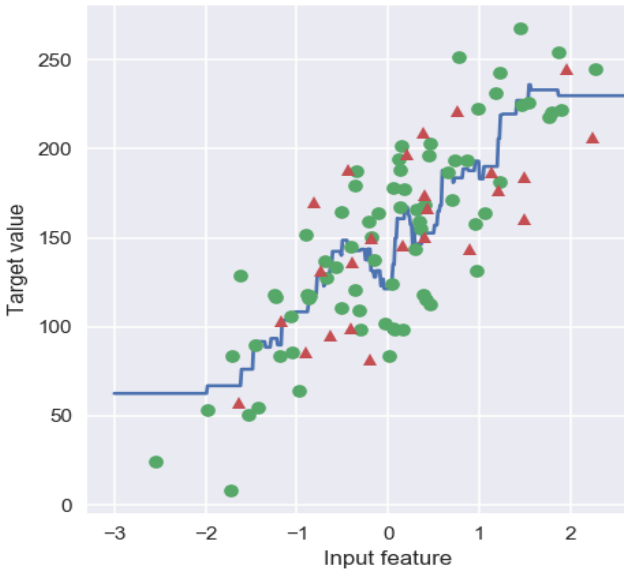
linreg.coef_ linreg.intercept_

$$\hat{y} = \boldsymbol{w_0} x_0 + b$$

K-NN Regression vs Least-Squares Linear Regression

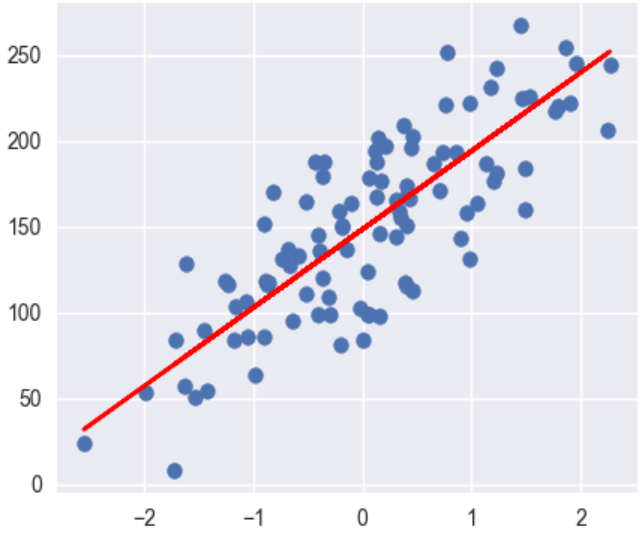
k-NN (k=7)

```
R-squared score (training): 0.720
R-squared score (test): 0.471
```



LS linear

```
R-squared score (training): 0.679
R-squared score (test): 0.492
```



Applied Machine Learning

Linear Regression:
Ridge, Lasso, and Polynomial Regression

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Ridge Regression

- **Ridge regression learns *w*, *b* using the same least-squares criterion but adds a penalty for large variations in *w* parameters**

$$RSS_{RIDGE}(\boldsymbol{w}, b) = \sum_{\{i=1\}}^{N} (\boldsymbol{y}_i - (\boldsymbol{w} \cdot \boldsymbol{x}_i + b))^2 + \alpha \sum_{\{j=1\}}^{p} w_j^2$$

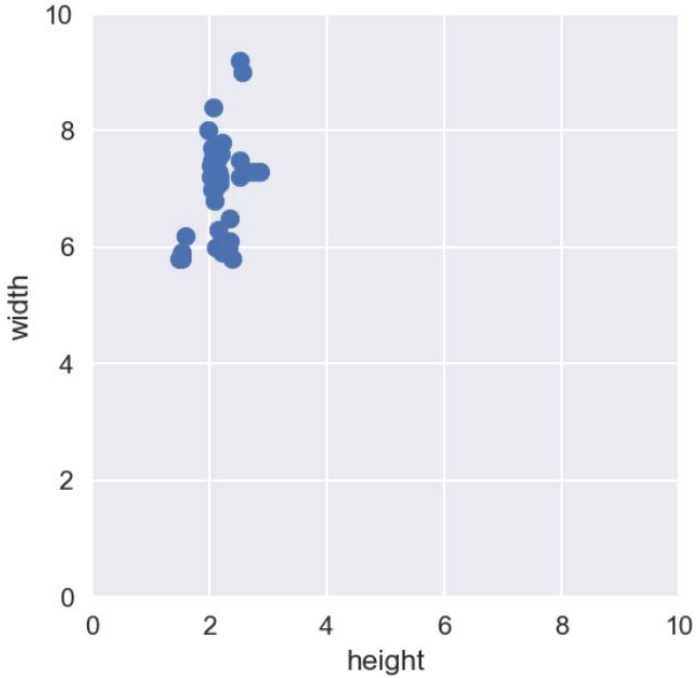
- **Once the parameters are learned, the ridge regression prediction formula is the same as ordinary least-squares.**
- **The addition of a parameter penalty is called regularization. Regularization prevents overfitting by restricting the model, typically to reduce its complexity.**
- **Ridge regression uses L2 regularization: minimize sum of squares of *w* entries**
- **The influence of the regularization term is controlled by the α parameter.**
- **Higher alpha means more regularization and simpler models.**

The Need for Feature Normalization

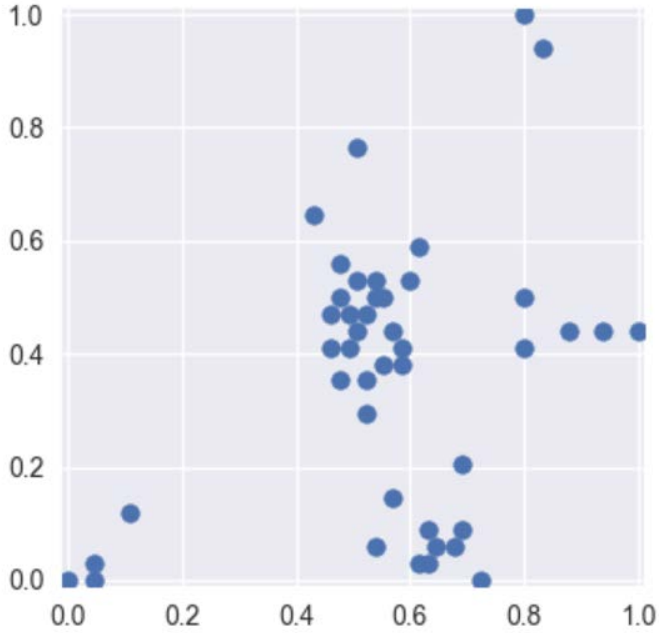
- **Important for some machine learning methods that all features are on the same scale (e.g. faster convergence in learning, more uniform or 'fair' influence for all weights)**
  - *e.g. regularized regression, k-NN, support vector machines, neural networks, …*
- **Can also depend on the data. More on feature engineering later in the course. For now, we do MinMax scaling of the features:**
  - *For each feature x_i : compute the min value x_i^{MIN} and the max value x_i^{MAX} achieved across all instances in the training set.*
  - *For each feature: transform a given feature x_i value to a scaled version x_i' using the formula*

$$x_i' = (x_i - x_i^{MIN})/(x_i^{MAX} - x_i^{MIN})$$

Feature Normalization with MinMaxScaler



Unnormalized data points



Normalized with MinMaxScaler

Using a scaler object: fit and transform methods

```
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
clf = Ridge().fit(X_train_scaled, y_train)
r2_score = clf.score(X_test_scaled, y_test)
```

Tip: It can be more efficient to do fitting and transforming together on the training set using the `fit_transform` method.

```
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
```

Feature Normalization: The test set must use identical scaling to the training set

- **Fit the scaler using the training set, then apply the same scaler to transform the test set.**
- **Do not scale the training and test sets using different scalers: this could lead to random skew in the data.**
- **Do not fit the scaler using any part of the test data: referencing the test data can lead to a form of *data leakage.* More on this issue later in the course.**

Lasso regression is another form of regularized linear regression that uses an L1 regularization penalty for training (instead of ridge's L2 penalty)

- **L1 penalty: Minimize the sum of the absolute values of the coefficients**

$$RSS_{LASSO}(\boldsymbol{w}, b) = \sum_{\{i=1\}}^{N} (\boldsymbol{y}_i - (\boldsymbol{w} \cdot \boldsymbol{x}_i + b))^2 + \alpha \sum_{\{j=1\}}^{p} |w_j|$$

- **This has the effect of setting parameter weights in *w* to zero for the least influential variables. This is called a sparse solution: a kind of feature selection**
- **The parameter α controls amount of L1 regularization (default = 1.0).**
- **The prediction formula is the same as ordinary least-squares.**
- **When to use ridge vs lasso regression:**
  - *Many small/medium sized effects: use ridge.*
  - *Only a few variables with medium/large effect: use lasso.*

Lasso Regression on the Communities and Crime Dataset

For alpha = 2.0, 20 out of 88 features have non-zero weight.

Top features (sorted by abs. magnitude):

```
PctKidsBornNeverMar, 1488.365 # percentage of kids born to people who never married
PctKids2Par, -1188.740 # percentage of kids in family housing with two parents
HousVacant, 459.538  # number of vacant households
PctPersDenseHous, 339.045 # percent of persons in dense housing (more than 1 person/room)
NumInShelters, 264.932 # number of people in homeless shelters
```

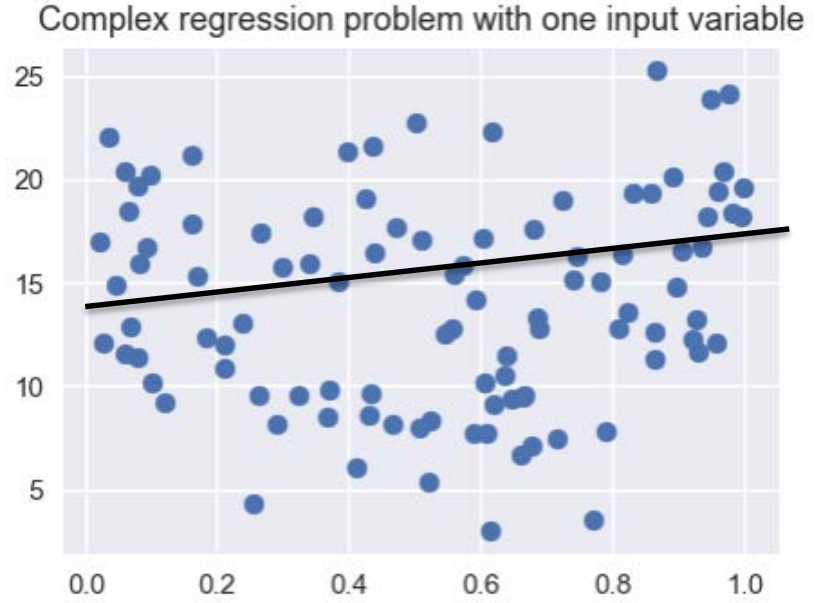
Polynomial Features with Linear Regression

$$\boldsymbol{x} = (x_0, x_1) \Rightarrow \boldsymbol{x}' = (x_0, x_1, x_0^2, x_0 x_1, x_1^2)$$

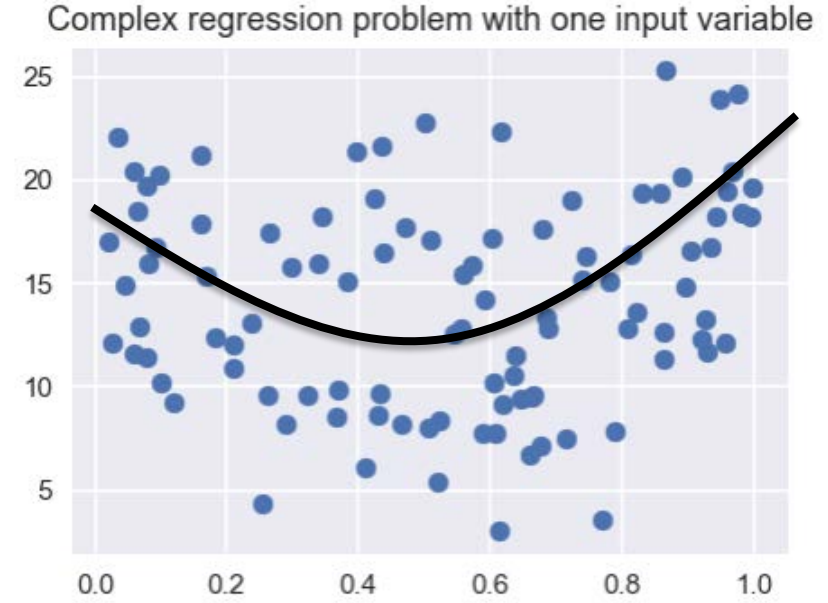
$$\hat{y} = \hat{w}_0 x_0 + \hat{w}_1 x_1 + \hat{w}_{00}\, x_0^2 + \hat{w}_{01} x_0 x_1 + \hat{w}_{11} x_1^2 + b$$

- **Generate new features consisting of all polynomial combinations of the original two features (x_0, x_1).**
- **The *degree* of the polynomial specifies how many variables participate at a time in each new feature (above example: degree 2)**
- **This is still a weighted linear combination of features, so it's still a linear model, and can use same least-squares estimation method for *w* and *b*.**

Least-Squares Polynomial Regression



Original feature



With polynomial degree 2 (quadratic) feature

Polynomial Features with Linear Regression

- **Why would we want to transform our data this way?**
  - *To capture interactions between the original features by adding them as features to the linear model.*
  - *To make a classification problem easier (we'll see this later).*
- **More generally, we can apply other non-linear transformations to create new features**
  - *(Technically, these are called non-linear basis functions)*
- **Beware of polynomial feature expansion with high as this can lead to complex models that overfit**
  - *Thus, polynomial feature expansion is often combined with a regularized learning method like ridge regression.*

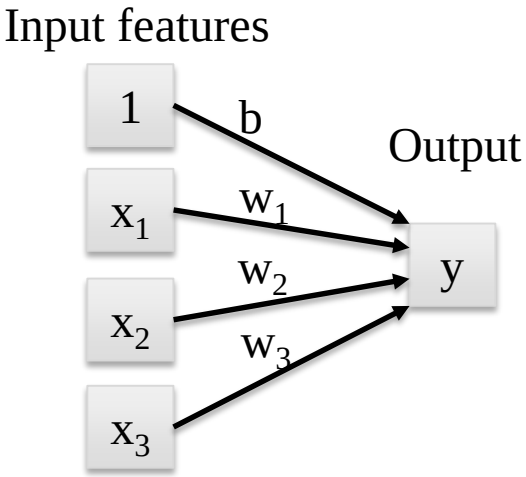
Applied Machine Learning

Logistic regression

Kevyn Collins-Thompson

Associate Professor of Information & Computer Science
University of Michigan

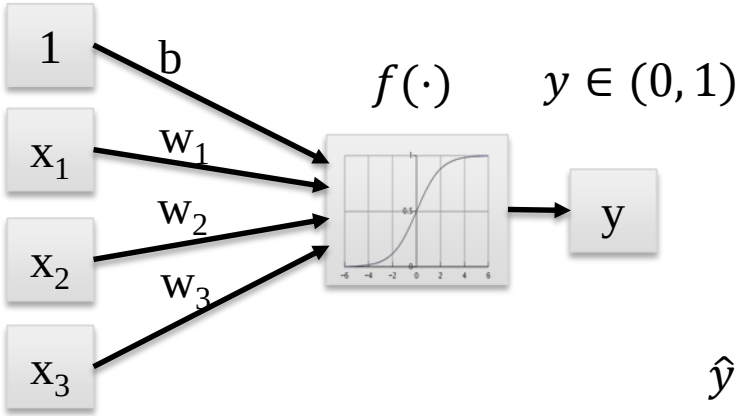
Linear Regression

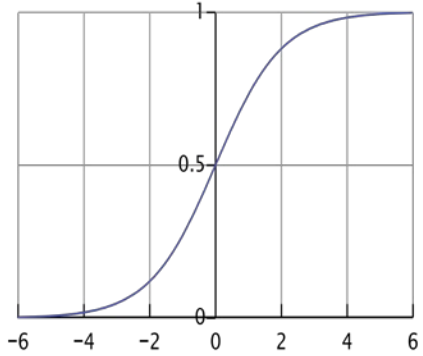


$$\hat{y} = \hat{b} + \hat{w}_1 \cdot x_1 + \cdots \hat{w}_n \cdot x_n$$

Linear models for classification: Logistic Regression

Input features



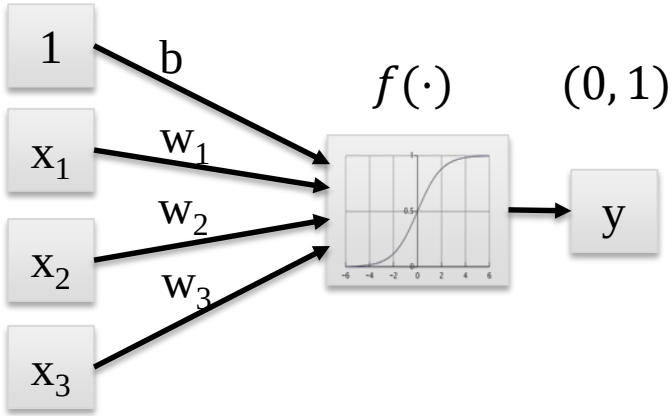


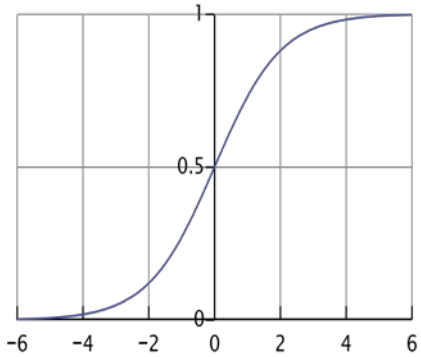
$$\hat{y} = \text{logistic}(\hat{b} + \hat{w}_1 \cdot x_1 + \cdots \hat{w}_n \cdot x_n)$$

$$= \frac{1}{1 + \exp\left[-(\hat{b} + \hat{w}_1 \cdot x_1 + \cdots \hat{w}_n \cdot x_n)\right]}$$

Linear models for classification: Logistic Regression

Input features



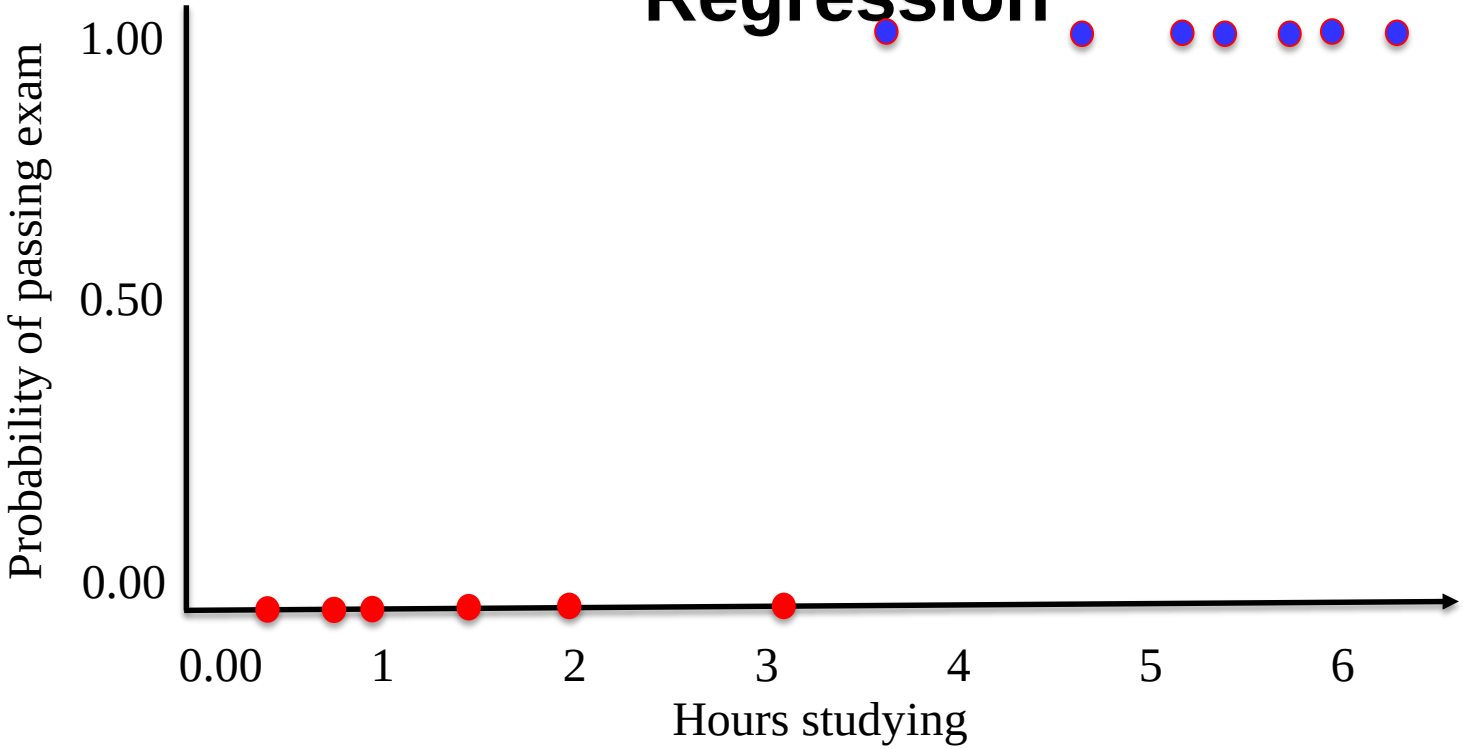


The logistic function transforms real-valued input to an output number *y* between 0 and 1, interpreted as the probability the input object belongs to the positive class, given its input features $(x_0, x_1, \ldots, x_n)$

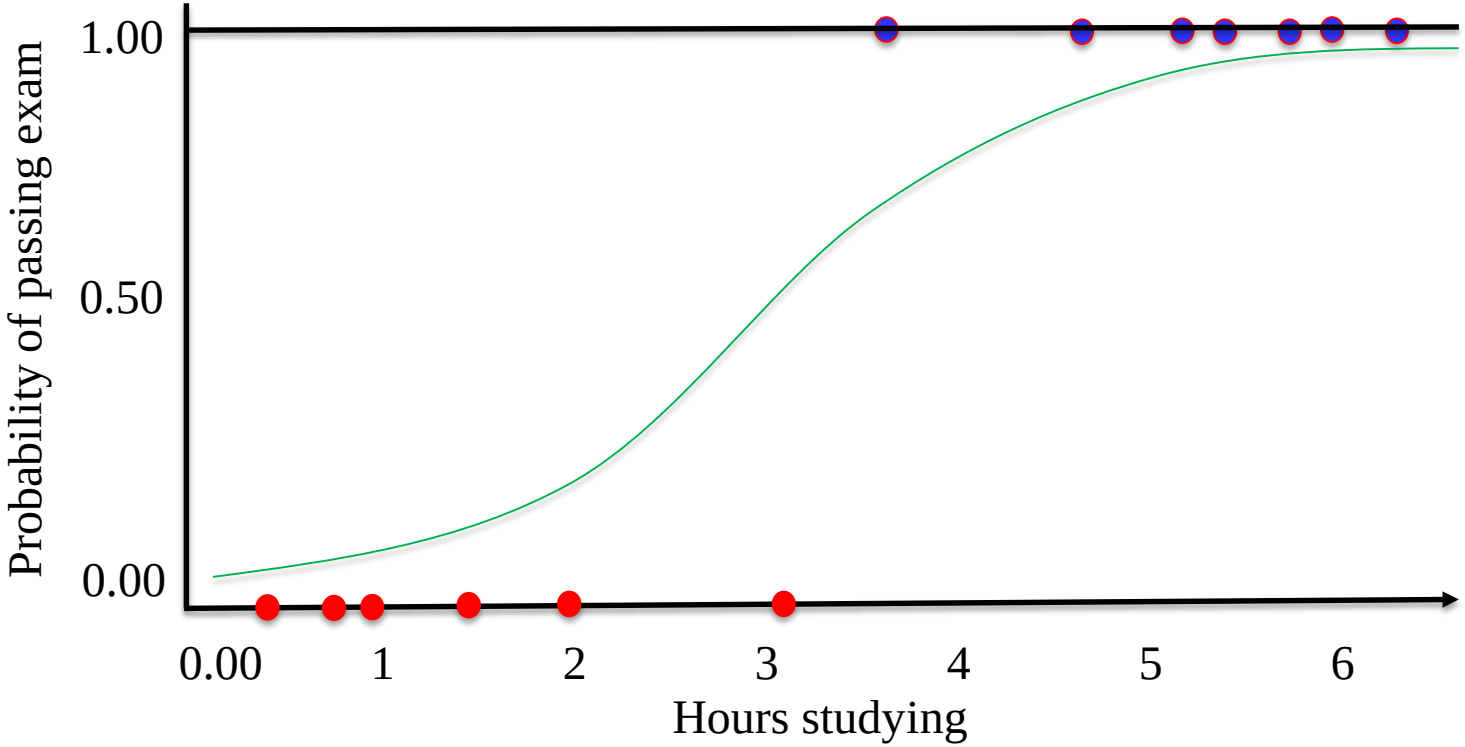
$$\hat{y} = \text{logistic}(\hat{b} + \hat{w}_1 \cdot x_1 + \cdots \hat{w}_n \cdot x_n)$$

$$= \frac{1}{1 + \exp\left[-(\hat{b} + \hat{w}_1 \cdot x_1 + \cdots \hat{w}_n \cdot x_n)\right]}$$

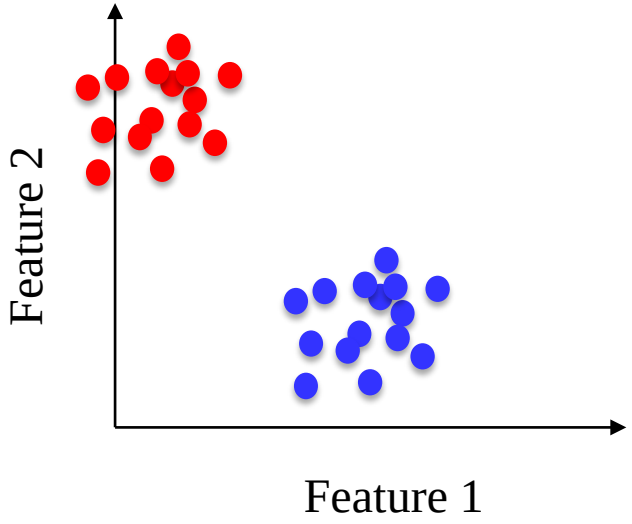
Linear models for classification: Logistic Regression



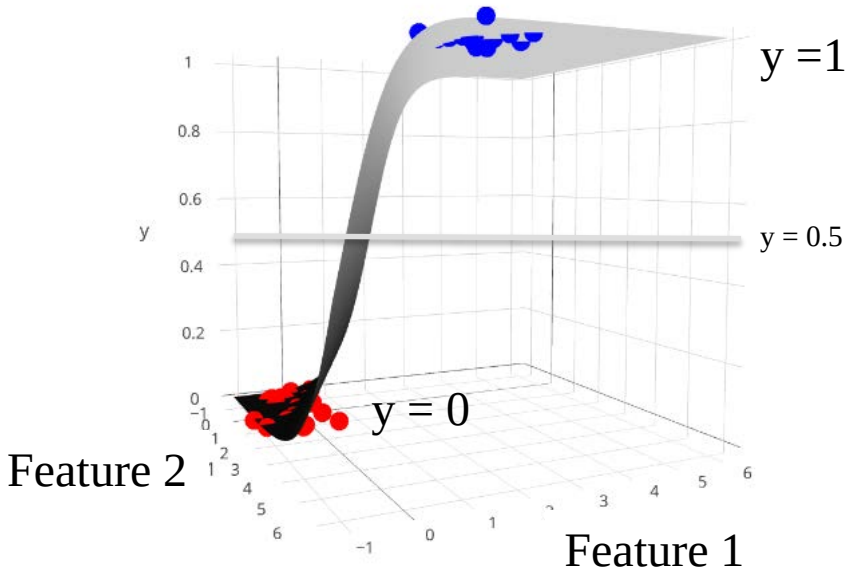
Linear models for classification: Logistic Regression



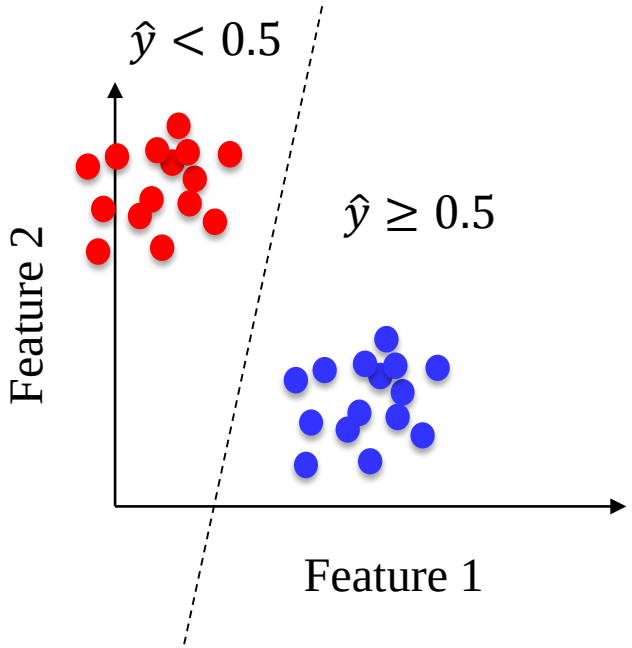
Logistic Regression for binary classification



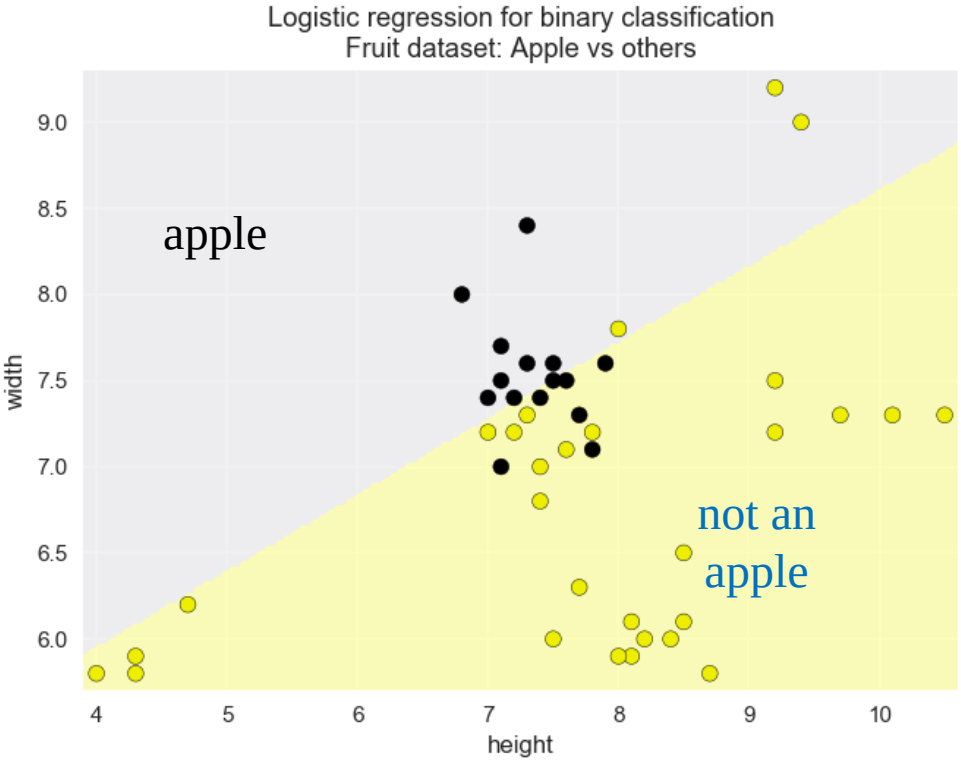
Logistic Regression for binary classification



Logistic Regression for binary classification

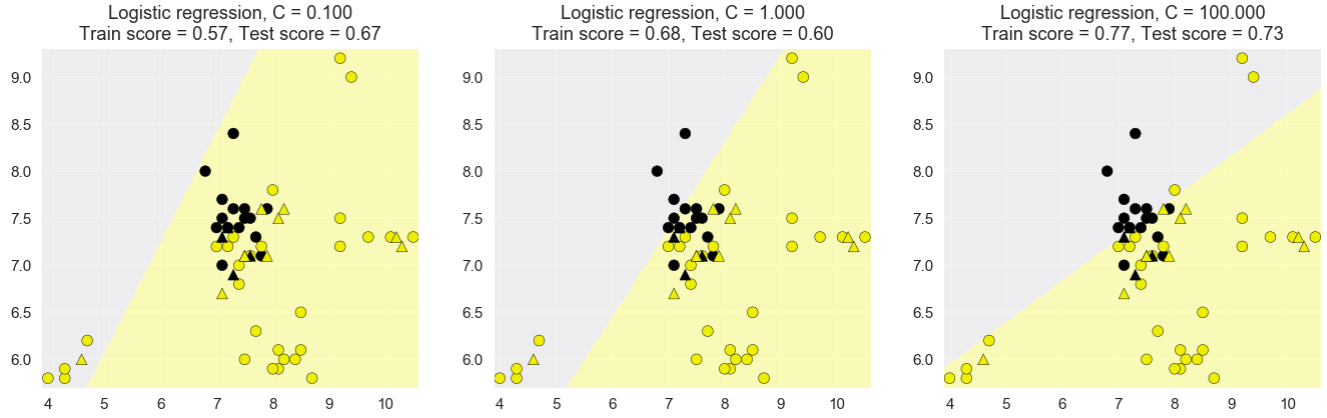


Simple logistic regression problem: two-class, two-feature version of the fruit dataset



Logistic Regression: Regularization

- L2 regularization is 'on' by default (like ridge regression)
- Parameter C controls amount of regularization (default 1.0)
- As with regularized linear regression, it can be important to normalize all features so that they are on the same scale.



Applied Machine Learning

Linear Classifiers:
Support Vector Machines

Kevyn Collins-Thompson

Associate Professor of Information & Computer Science
University of Michigan

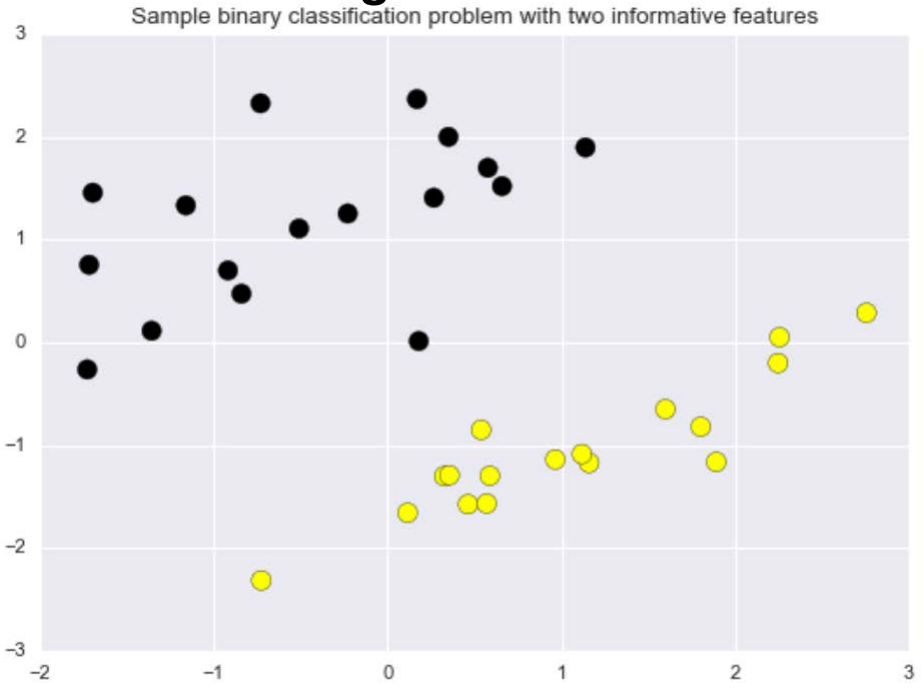
Linear classifiers: how would you separate these two groups of training examples with a straight line?

Feature vector

Class value

$$f(x, w, b) = sign(w \circ x + b)$$

$$= sign\left(\sum w[i]x[i] + b\right)$$



Linear classifiers: how would you separate these two groups of training examples with a straight line?

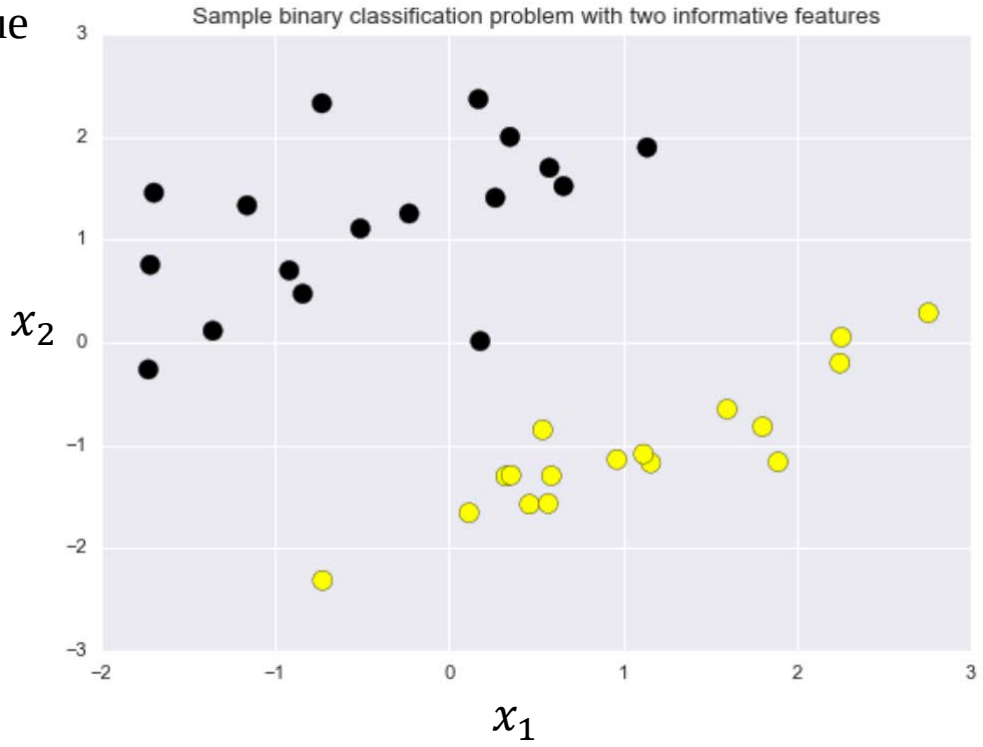
Feature vector

$\boldsymbol{x} = (x_1, x_2)$ → f → $\hat{y}$

Class value

$$f(\boldsymbol{x}, w, b) = sign(w \circ \boldsymbol{x} + b)$$

A linear classifier is a function that maps an input data point *x* to an output class value *y* (+1 or -1) using a linear function (with weight parameters *w* of the input point's features.



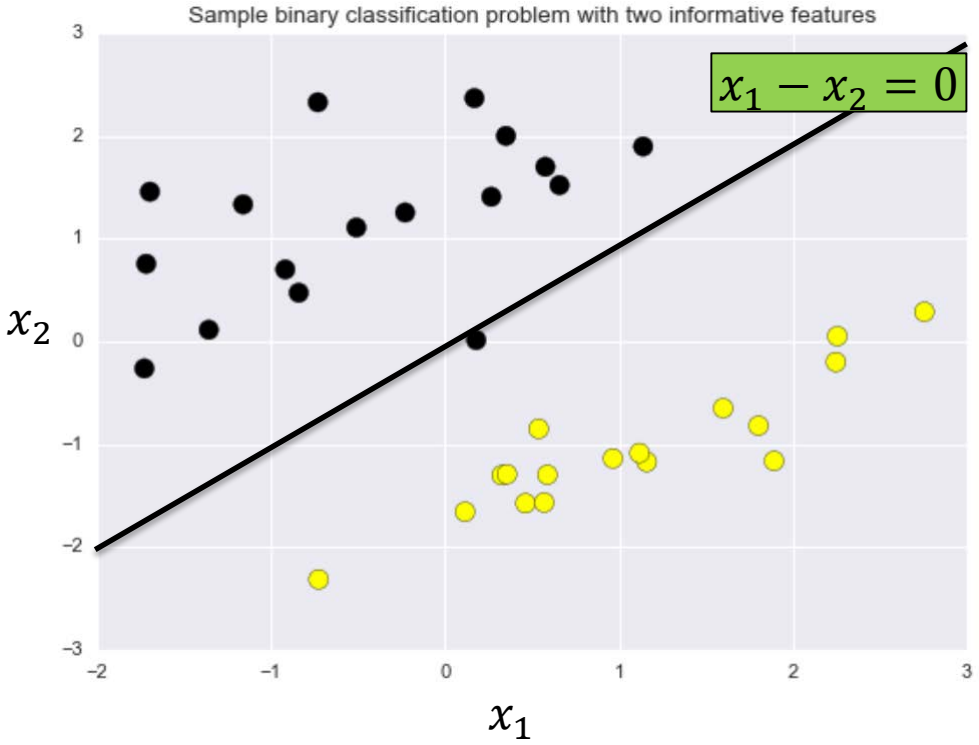
Linear classifiers: how would you separate these two groups of training examples with a line?

Feature vector

Class value

$$f(x, w, b) = sign(w \circ x + b)$$

$$x_1 - x_2 = 0$$
$$w = [1, -1]$$
$$b = 0$$



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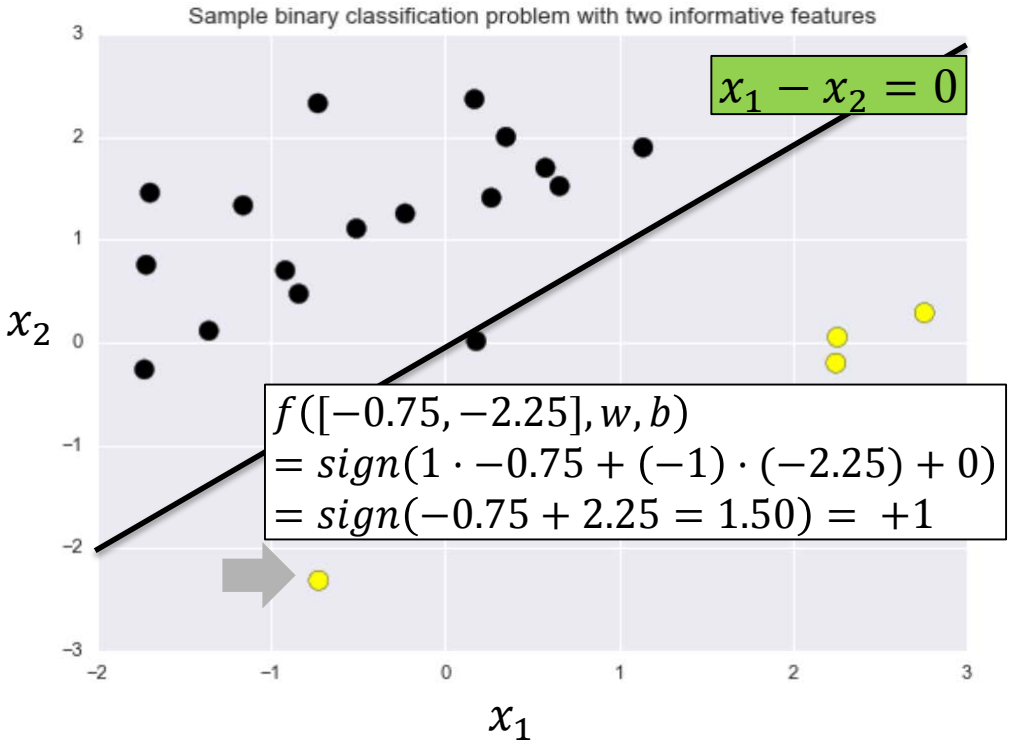

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Feature vector

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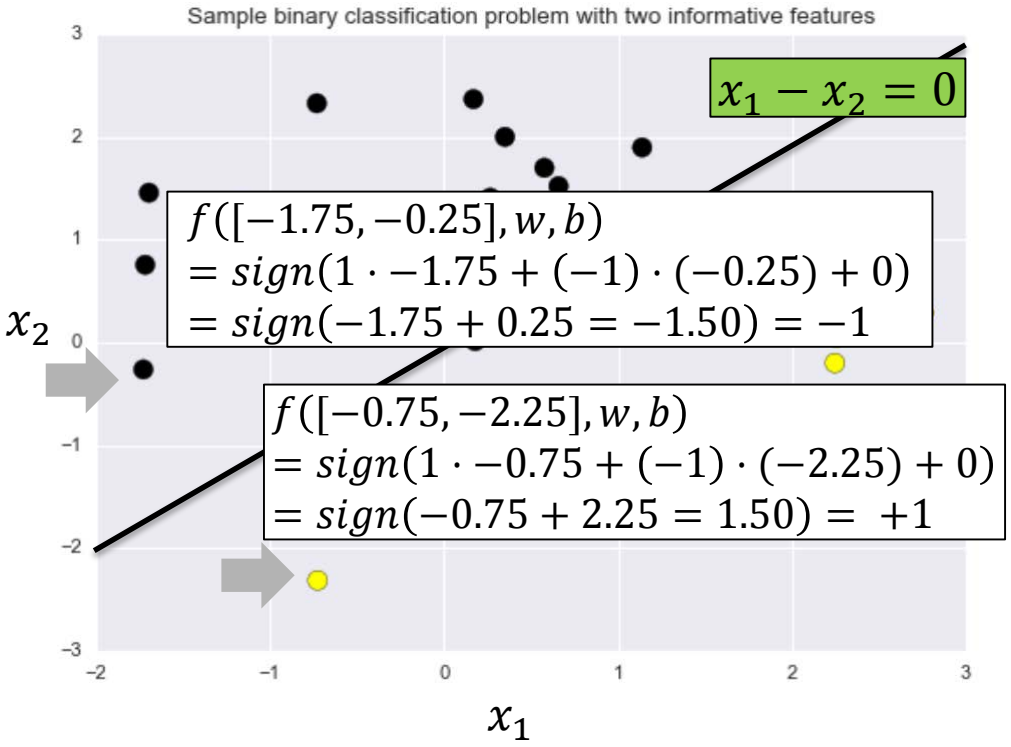
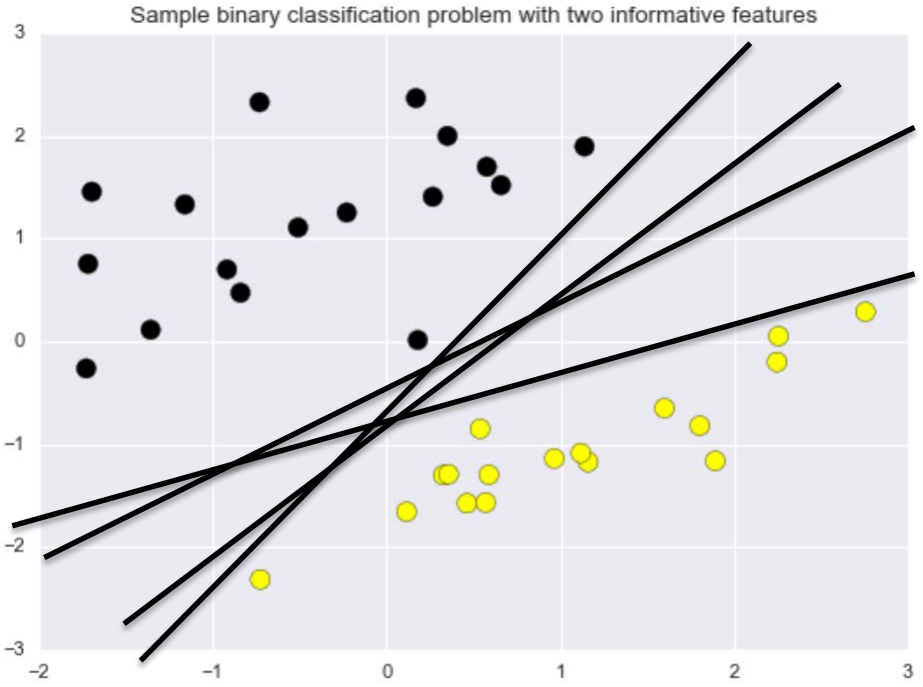


Linear Classifiers

$$f(x, w, b) = sign(w \circ x + b)$$

There are many possible linear classifiers that could separate the two classes.
Which one is best?

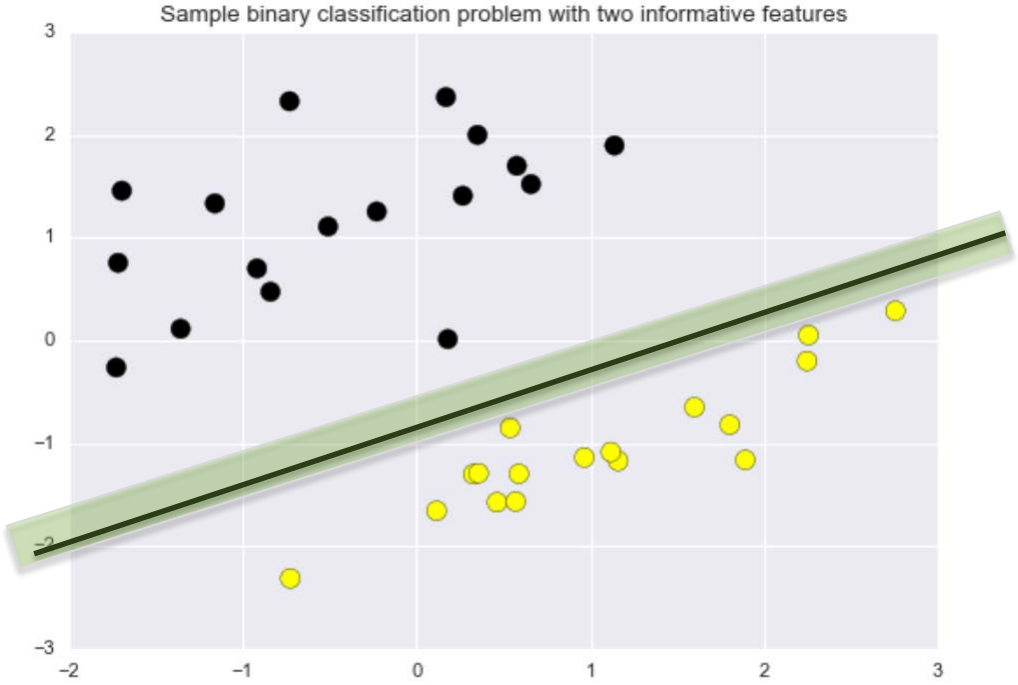


Classifier Margin

$$f(x, w, b) = sign(w \circ x + b)$$

Classifier margin

Defined as the maximum width the decision boundary area can be increased before hitting a data point.

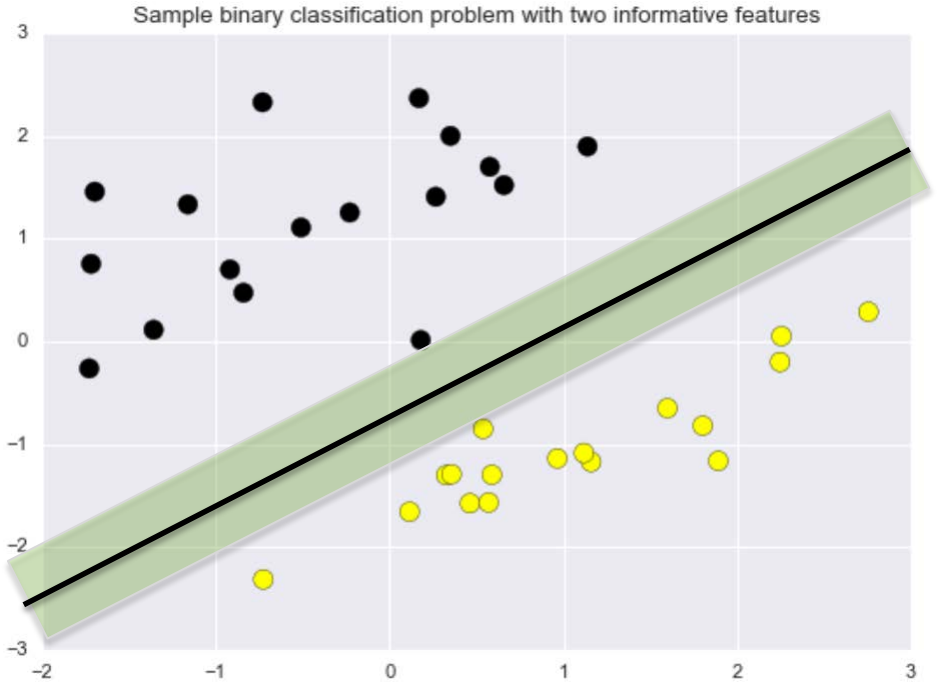


Maximum margin linear classifier: Linear Support Vector Machines

$$f(x, w, b) = sign(w \circ x + b)$$

Maximum margin classifier

The linear classifier with maximum margin is a linear Support Vector Machine (LSVM).



Regularization for SVMs: the C parameter

- **The strength of regularization is determined by C**
- **Larger values of C: less regularization**
  - *Fit the training data as well as possible*
  - *Each individual data point is important to classify correctly*
- **Smaller values of C: more regularization**
  - *More tolerant of errors on individual data points*

Linear Models: Pros and Cons

Pros:

- Simple and easy to train.
- Fast prediction.
- Scales well to very large datasets.
- Works well with sparse data.
- Reasons for prediction are relatively easy to interpret.

Cons:

- For lower-dimensional data, other models may have superior generalization performance.
- For classification, data may not be linearly separable (more on this in SVMs with non-linear kernels)

linear_model: Important Parameters

Model complexity

- **alpha: weight given to the L1 or L2 regularization term in regression models**
  - *default = 1.0*
- **C: regularization weight for LinearSVC and LogisticRegression classification models**
  - *default = 1.0*

Applied Machine Learning

Multi-Class Classification

Kevyn Collins-Thompson

Associate Professor of Information & Computer Science
University of Michigan

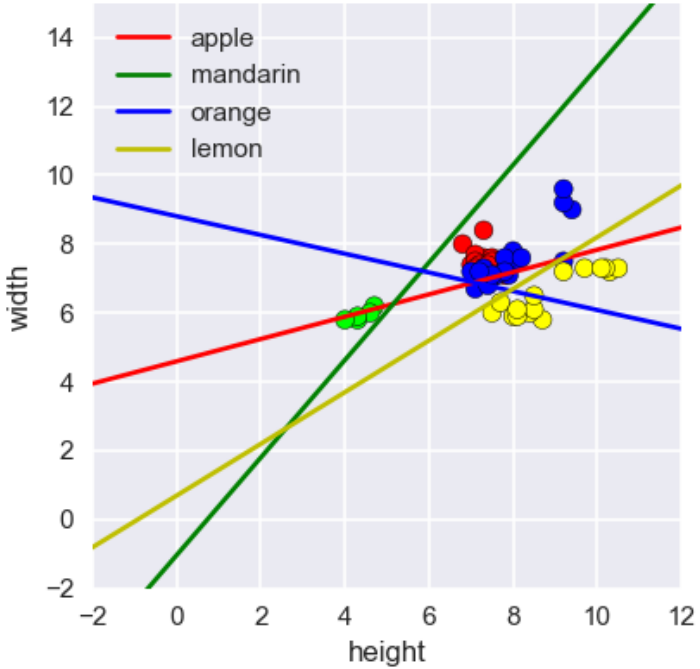
Multi-Class classification with linear models

```
clf = LinearSVC(C=5, random_state = 67)
clf.fit(X_train, y_train)

print(clf.coef_)

[[-0.23401135  0.72246132]
 [-1.63231901  1.15222281]
 [ 0.0849835   0.31186707]
 [ 1.26189663 -1.68097   ]]

print(clf.intercept_)
[-3.31753728  1.19645936 -2.7468353  1.16107418]
```



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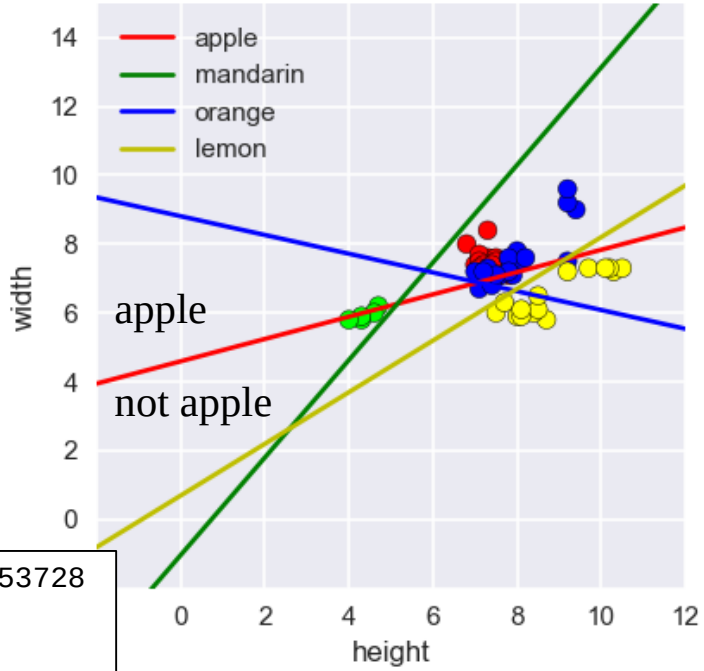



```
y_apple = -0.23401135 * height + 0.72246132 * width – 3.31753728

height=2, width=6:  y_apple = + 0.549 (>= 0: predict apple)
height=2, width=2:  y_apple = - 2.340 (< 0:  predict other)
```

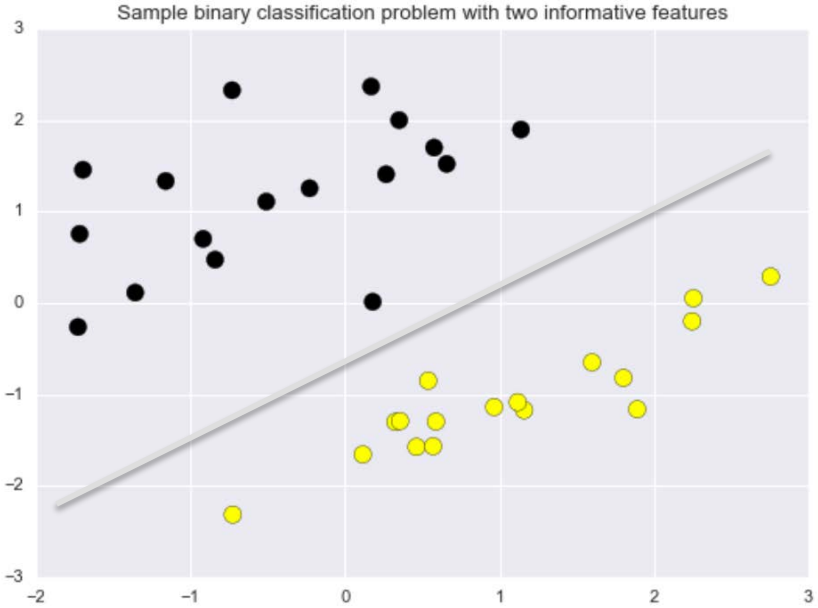
Applied Machine Learning

Kernelized Support Vector Machines

Kevyn Collins-Thompson

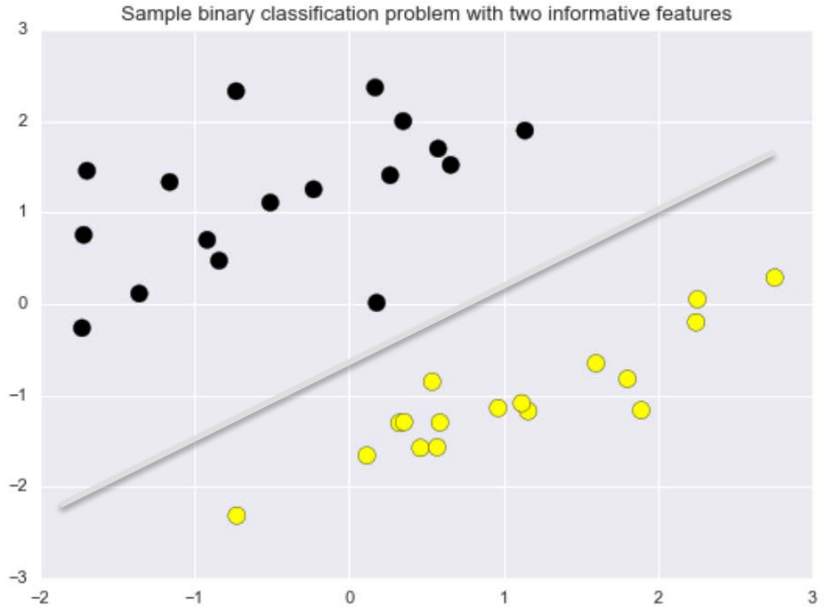
Associate Professor of Information & Computer Science
University of Michigan

We saw how linear support vector classifiers could effectively find a decision boundary with maximum margin

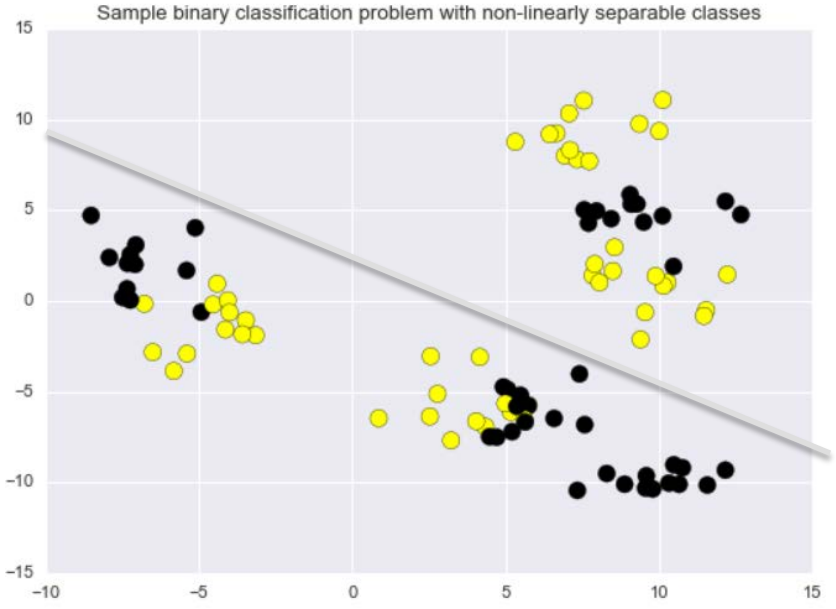


Easy for a linear classifier

But what about more complex binary classification problems?

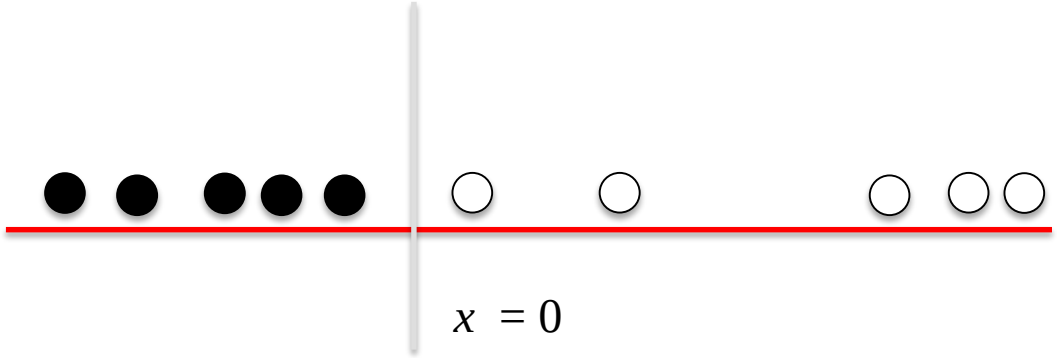


Easy for a linear classifier



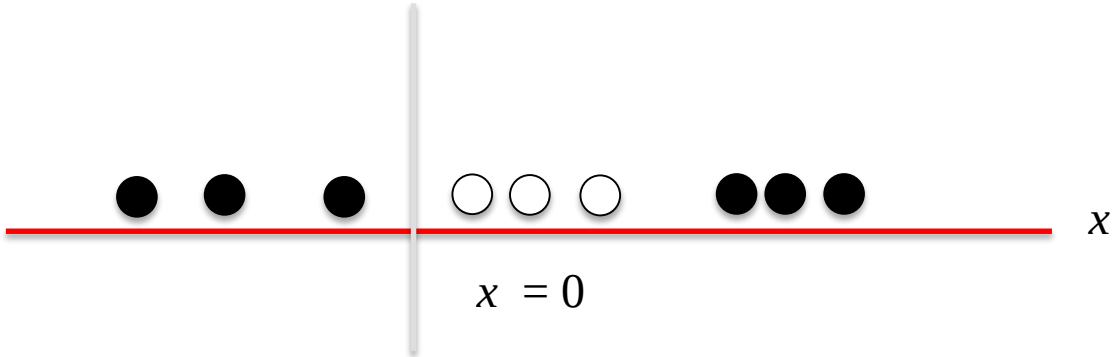
Difficult/impossible for a linear classifier

A simple 1-dimensional classification problem for a linear classifier

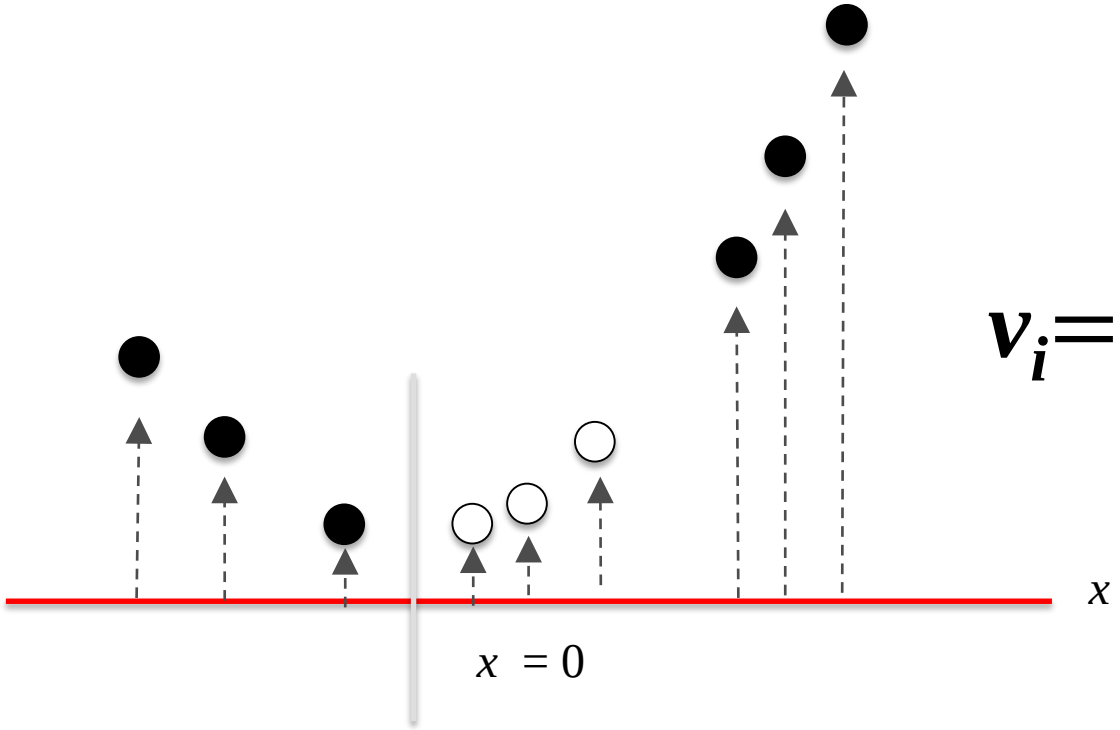


A more perplexing 1-d classification problem for a linear classifier

A more perplexing 1-d classification problem for a linear classifier

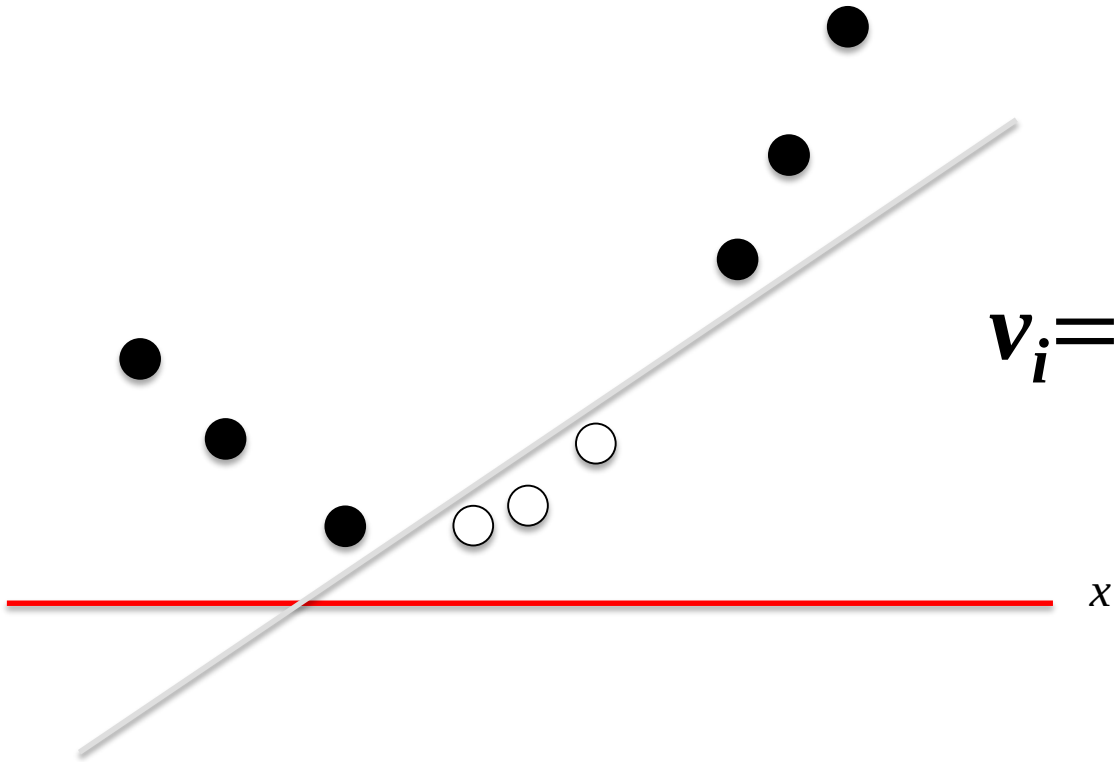


Let's transform the data by adding a second dimension/feature (set to the squared value of the first feature)



$$\boldsymbol{v_i} = (x_i, x_i^2)$$

The data transformation makes it possible to solve this with a linear classifier

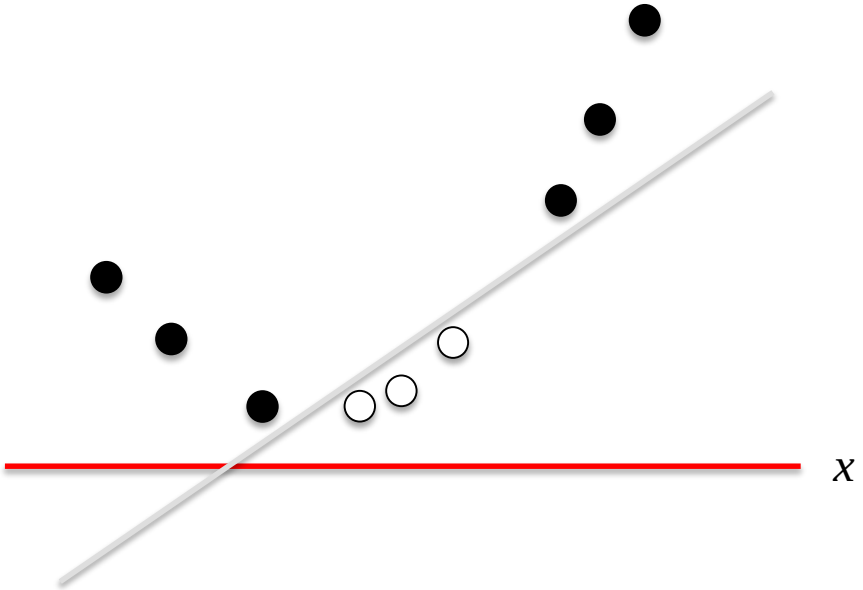


$$\boldsymbol{v_i} = (x_i, x_i^2)$$

What does the linear decision boundary in feature space correspond to in the original input space?

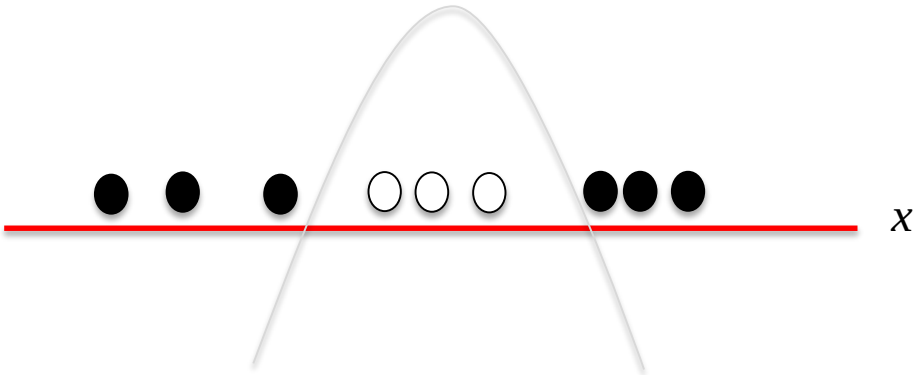
Original input space

Feature space

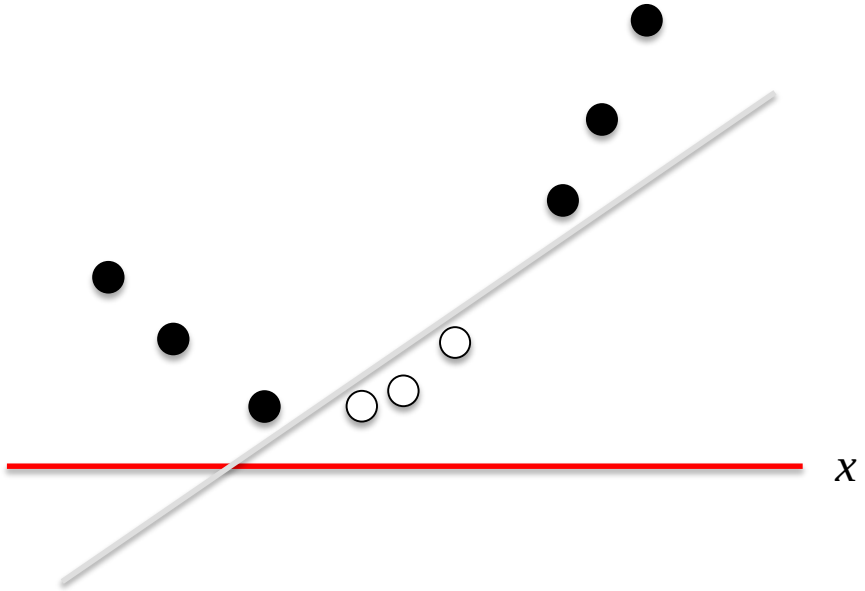


What does the linear decision boundary correspond to in the original input space?

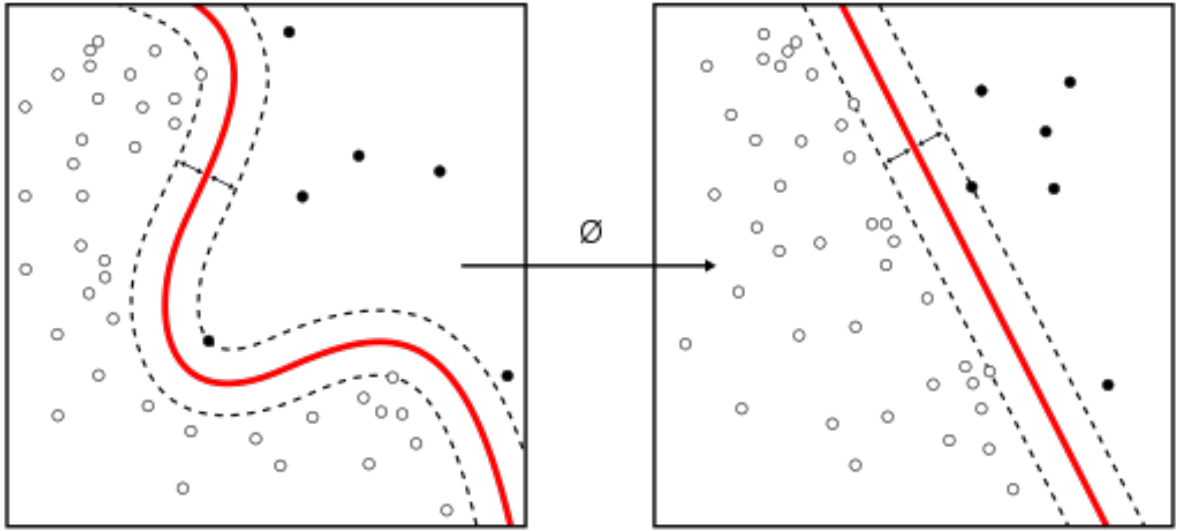
Original input space



Feature space



Transforming the data can make it much easier for a linear classifier.

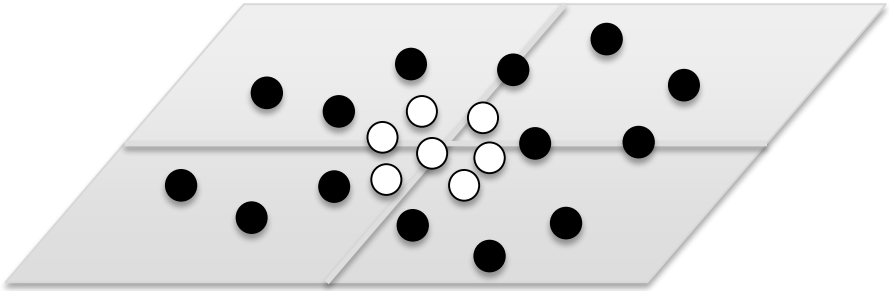


Original input space **Feature space**

Source: Wikipedia "Kernel Machine" article.
https://commons.wikimedia.org/w/index.php?curid=47868867

Example of mapping a 2D classification problem to a 3D feature space to make it linearly separable

Original input space

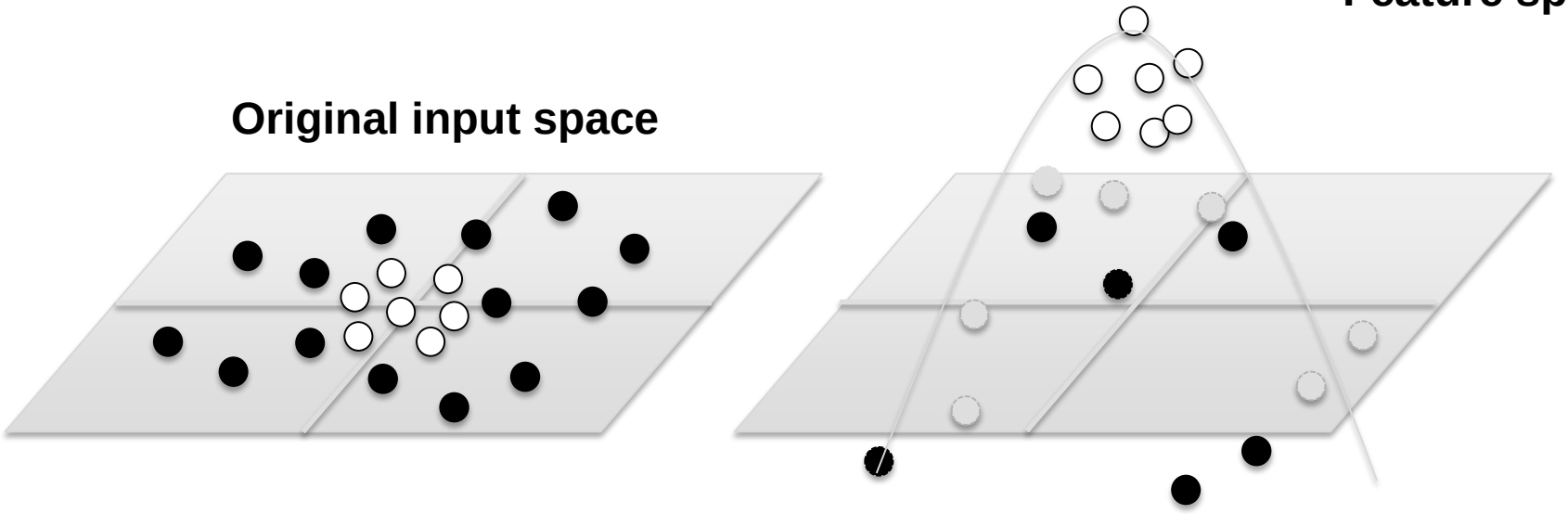


$$x_i = (x_0, x_1)$$

Example of mapping a 2D classification problem to a 3D feature space to make it linearly separable

Feature space

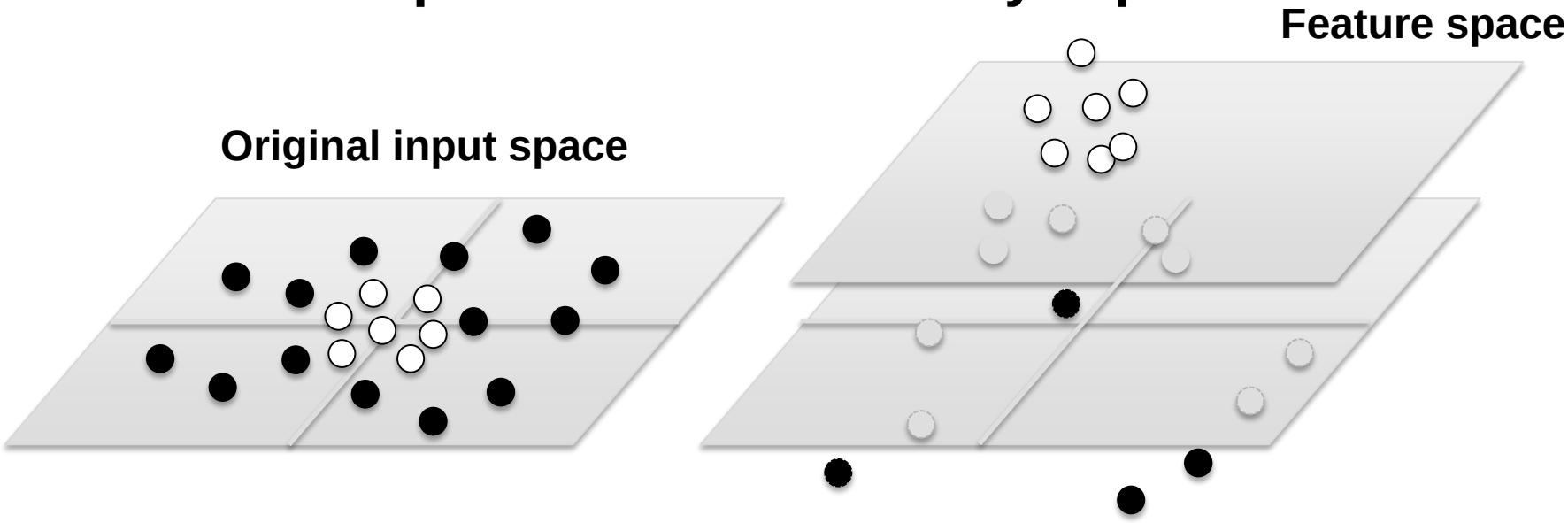
Original input space



$$\boldsymbol{x_i} = (x_0, x_1)$$

$$\boldsymbol{v_i} = (x_0, x_1, 1 - (x_0^2 + x_1^2))$$

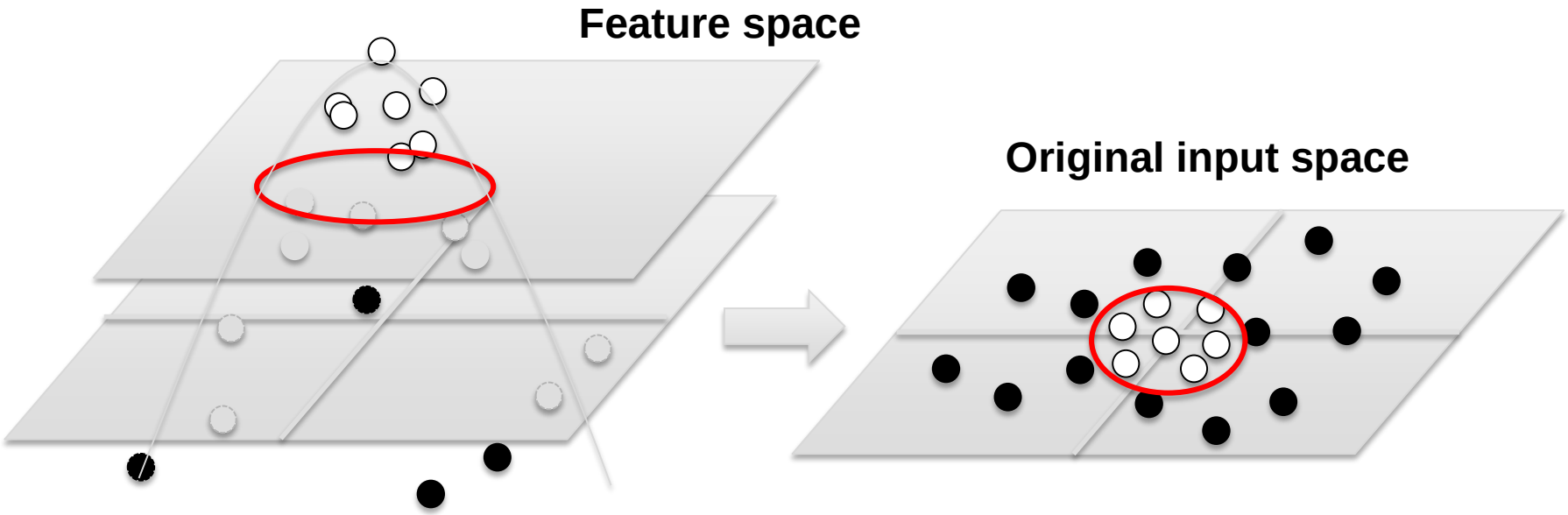
Example of mapping a 2D classification problem to a 3D feature space to make it linearly separable



$$\boldsymbol{x_i} = (x_0, x_1)$$

$$\boldsymbol{v_i} = (x_0, x_1, 1 - (x_0^2 + x_1^2))$$

Example of mapping a 2D classification problem to a 3D feature space to make it linearly separable

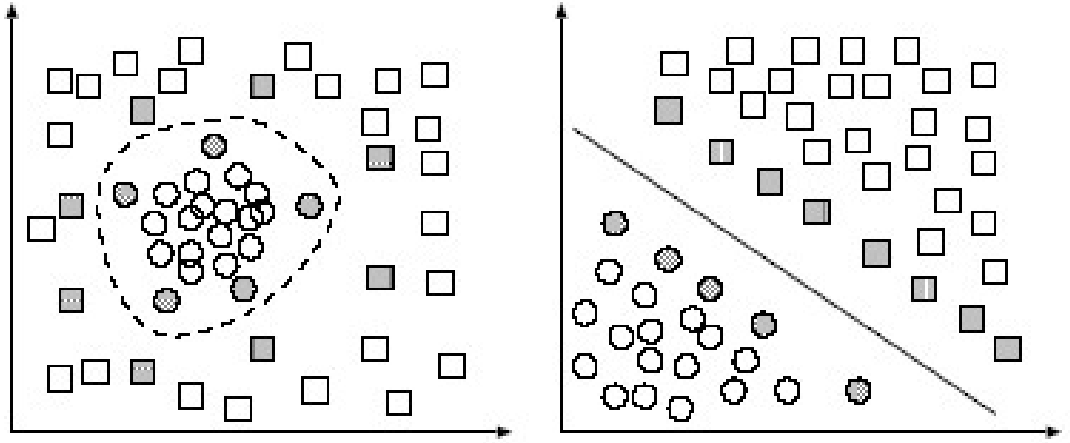


$$\boldsymbol{v_i} = (x_0, x_1, 1 - (x_0^2 + x_1^2))$$

$$\boldsymbol{x_i} = (x_0, x_1)$$

Radial Basis Function Kernel

$$K(\boldsymbol{x}, \boldsymbol{x}') = \exp\ [-\gamma \cdot \|\boldsymbol{x} - \boldsymbol{x}'\|^2]$$

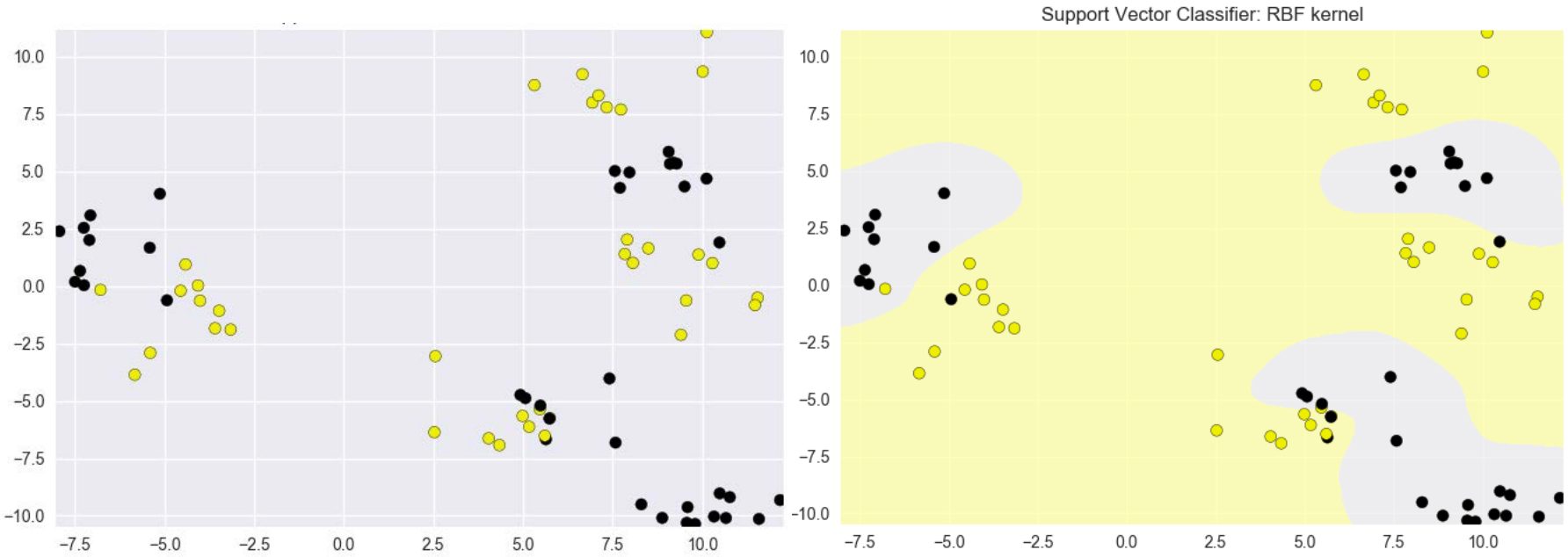


Original input space

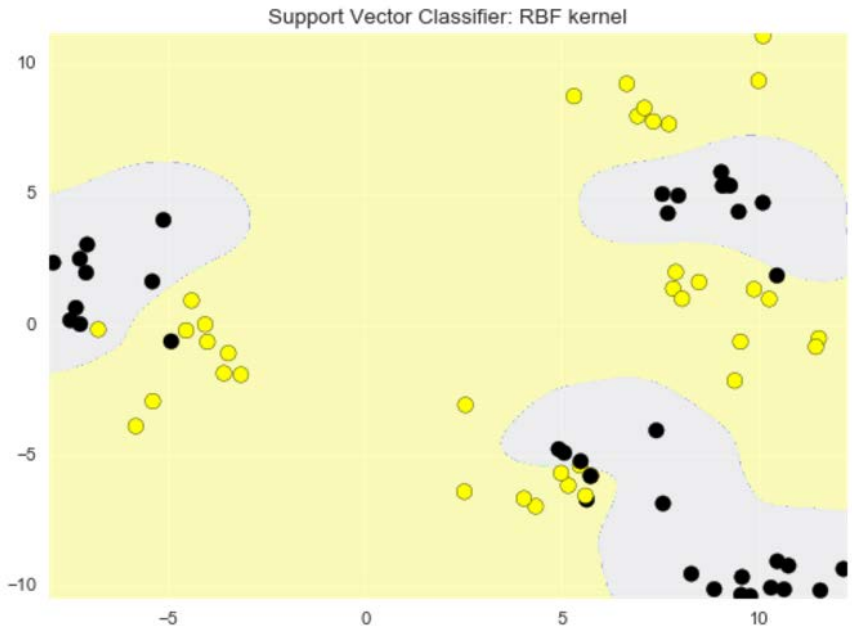
Feature space

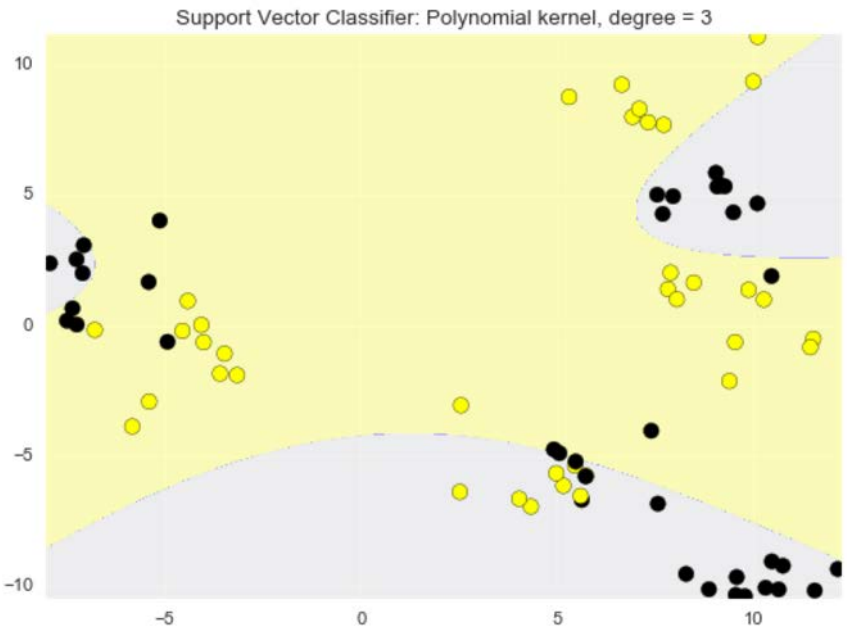
A kernel is a similarity measure (modified dot product) between data points

Applying the SVM with RBF kernel



Radial Basis Kernel vs Polynomial Kernel



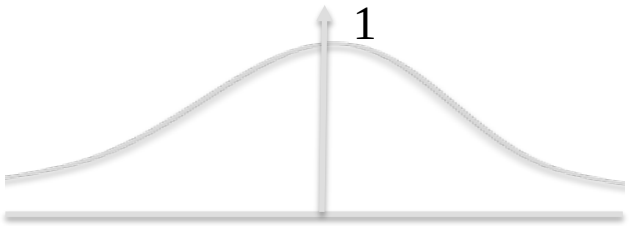


Radial Basis Function kernel: Gamma Parameter

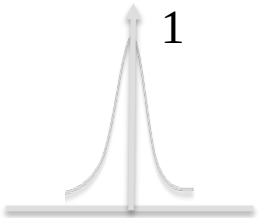
$$K(\boldsymbol{x}, \boldsymbol{x}') = \exp\ [-\gamma \cdot \|\boldsymbol{x} - \boldsymbol{x}'\|^2]$$

gamma (γ): kernel width parameter

small gamma (0.01)



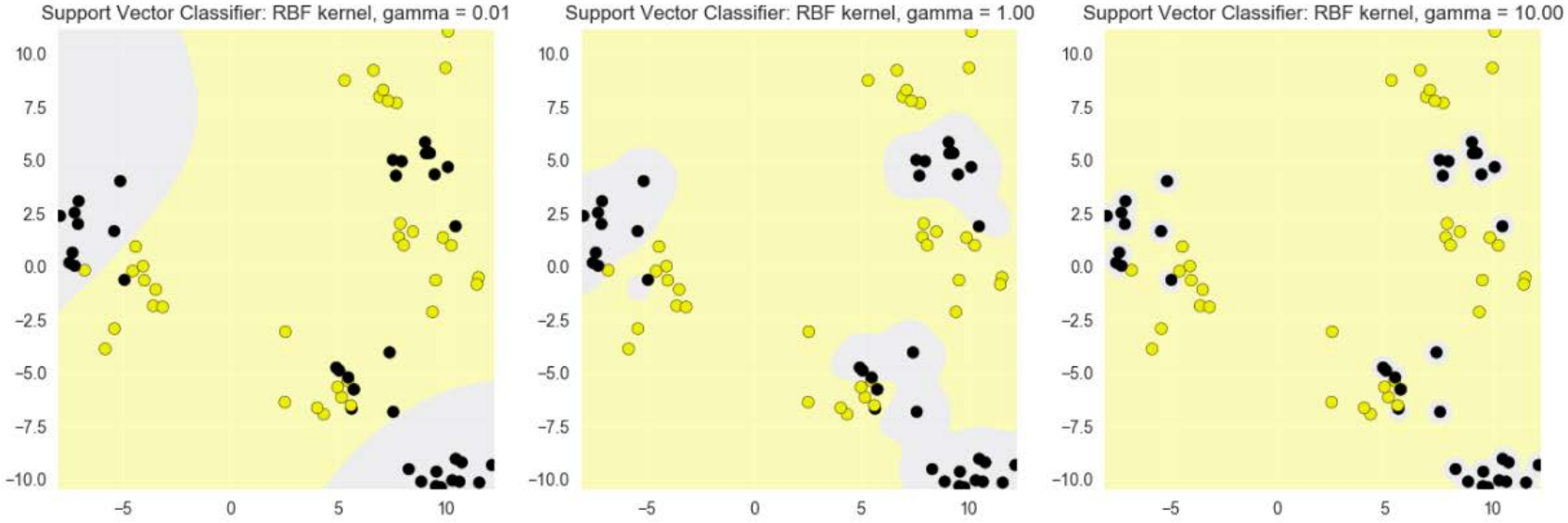
large gamma (10)



$\|\boldsymbol{x} - \boldsymbol{x}'\|^2$

Squared distance between x and x'

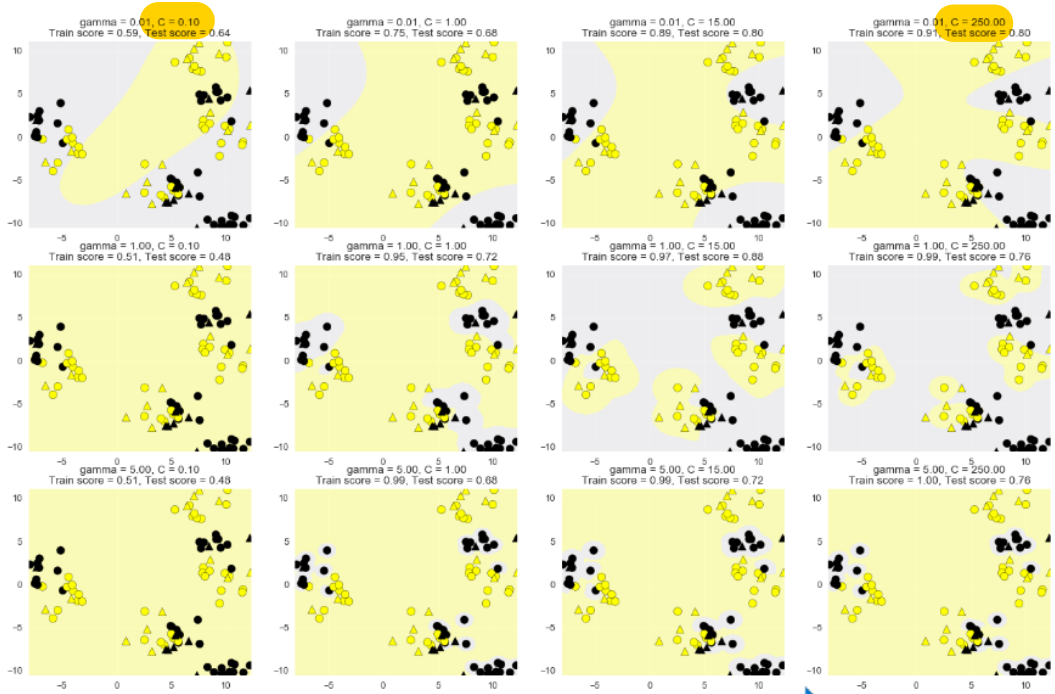
The effect of the RBF gamma parameter on decision boundaries



gamma = 0.01

gamma = 1.0

gamma = 10


gamma = 0.01, C = 0.10
Train score = 0.59, Test score = 0.64
gamma = 0.01, C = 1.00
Train score = 0.75, Test score = 0.68
gamma = 0.01, C = 15.00
Train score = 0.89, Test score = 0.80
gamma = 0.01, C = 250.00
Train score = 0.91, Test score = 0.80
gamma = 1.00, C = 0.10
Train score = 0.51, Test score = 0.48
gamma = 1.00, C = 1.00
Train score = 0.95, Test score = 0.72
gamma = 1.00, C = 15.00
Train score = 0.97, Test score = 0.88
gamma = 1.00, C = 250.00
Train score = 0.99, Test score = 0.76
gamma = 5.00, C = 0.10
Train score = 0.51, Test score = 0.48
gamma = 5.00, C = 1.00
Train score = 0.99, Test score = 0.68
gamma = 5.00, C = 15.00
Train score = 0.99, Test score = 0.72
gamma = 5.00, C = 250.00
Train score = 1.00, Test score = 0.76
Increasing gamma
Increasing C

Reminder: Using a scaler object: fit and transform methods

```
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
clf = SVC().fit(X_train_scaled, y_train)
accuracy = clf.score(X_test_scaled, y_test)
```

Tip: It can be more efficient to do fitting and transforming together on the training set using the `fit_transform` method.

```
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
```

Kernelized Support Vector Machines: pros and cons

Pros:

- Can perform well on a range of datasets.
- Versatile: different kernel functions can be specified, or custom kernels can be defined for specific data types.
- Works well for both low- and high-dimensional data.

Cons:

- Efficiency (runtime speed and memory usage) decreases as training set size increases (e.g. over 50000 samples).
- Needs careful normalization of input data and parameter tuning.
- Does not provide direct probability estimates (but can be estimated using e.g. Platt scaling).
- Difficult to interpret why a prediction was made.

Kernelized Support Vector Machines (SVC): Important parameters

Model complexity

- **`kernel`: Type of kernel function to be used**
  - *Default = 'rbf' for radial basis function*
  - *Other types include 'polynomial'*
- **kernel parameters**
  - `gamma` *(γ): RBF kernel width*
- **`C`: regularization parameter**
- **Typically `C` and `gamma` are tuned at the same time.**

Applied Machine Learning

Cross-validation

Kevyn Collins-Thompson

Associate Professor of Information & Computer Science
University of Michigan

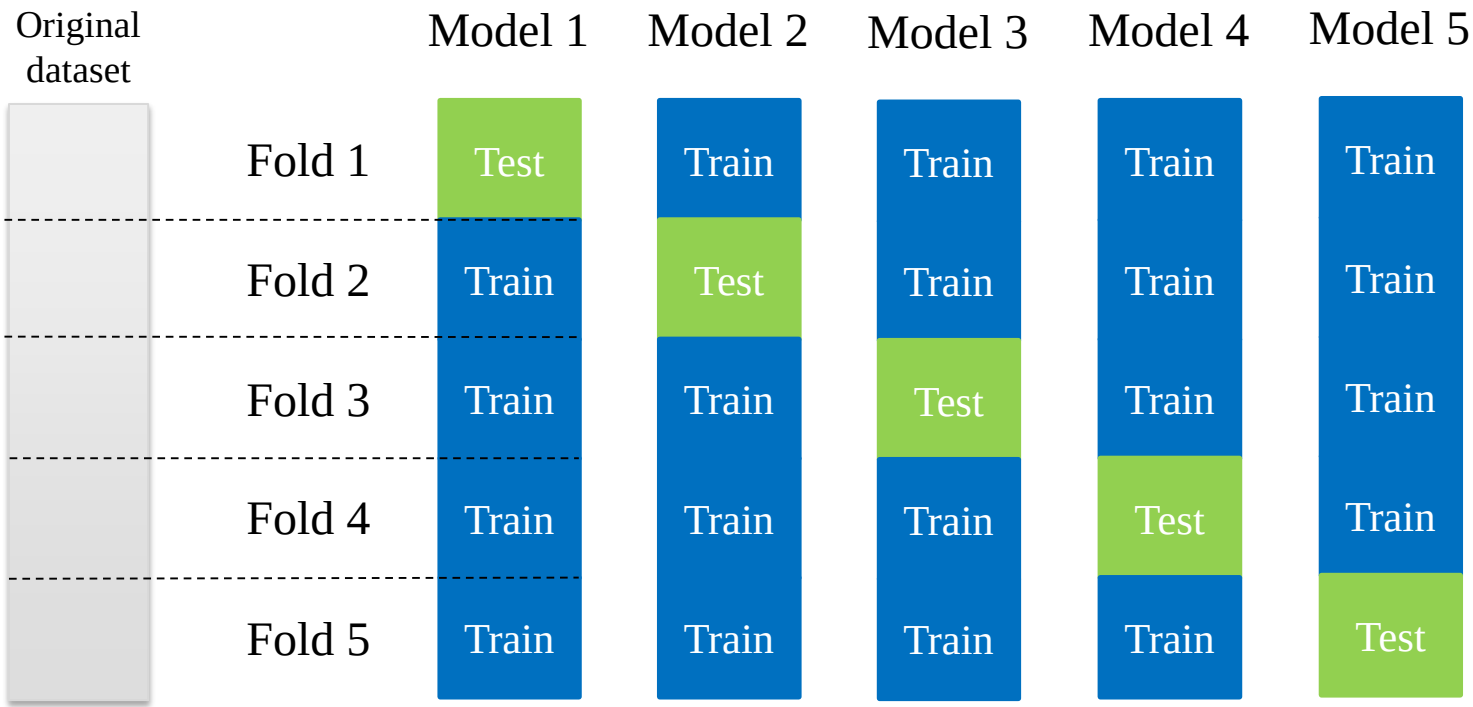
Cross-validation

- **Uses multiple train-test splits, not just a single one**
- **Each split used to train & evaluate a separate model**
- **Why is this better?**
  - *The accuracy score of a supervised learning method can vary, depending on which samples happen to end up in the training set.*
  - *Using multiple train-test splits gives more stable and reliable estimates for how the classifier is likely to perform on average.*
  - *Results are averaged over multiple different training sets instead of relying on a single model trained on a particular training set.*

random_state	Test set accuracy
0	1.00
1	0.93
5	0.93
7	0.67
10	0.87

Accuracy of k-NN classifier (k=5) on fruit data test set for different random_state values in train_test_split.

Cross-validation Example (5-fold)



Stratified Cross-validation

fruit_label	fruit_name
1	Apple
1	Apple
1	Apple
1	Apple
1	Apple
2	Mandarin
...	...
3	Orange
...	...
4	Lemon
4	Lemon
4	Lemon
4	Lemon
4	Lemon

(Folds and dataset shortened for illustration purposes.)

Example has 20 data samples
= 4 classes with 5 samples each.

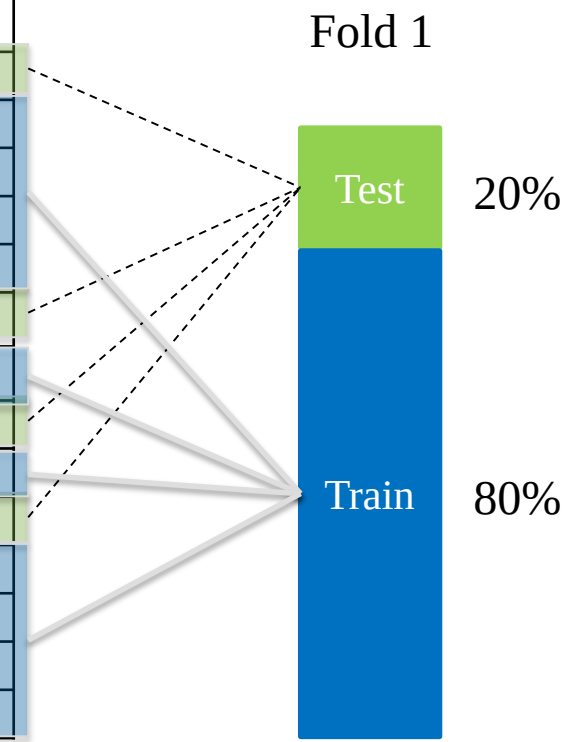
5-fold CV: 5 folds of 4 samples each.

Fold 1 uses the first 20% of the dataset as the test set, which only contains samples from class 1.

Classes 2, 3, 4 are missing entirely from test set and so will be missing from the evaluation.

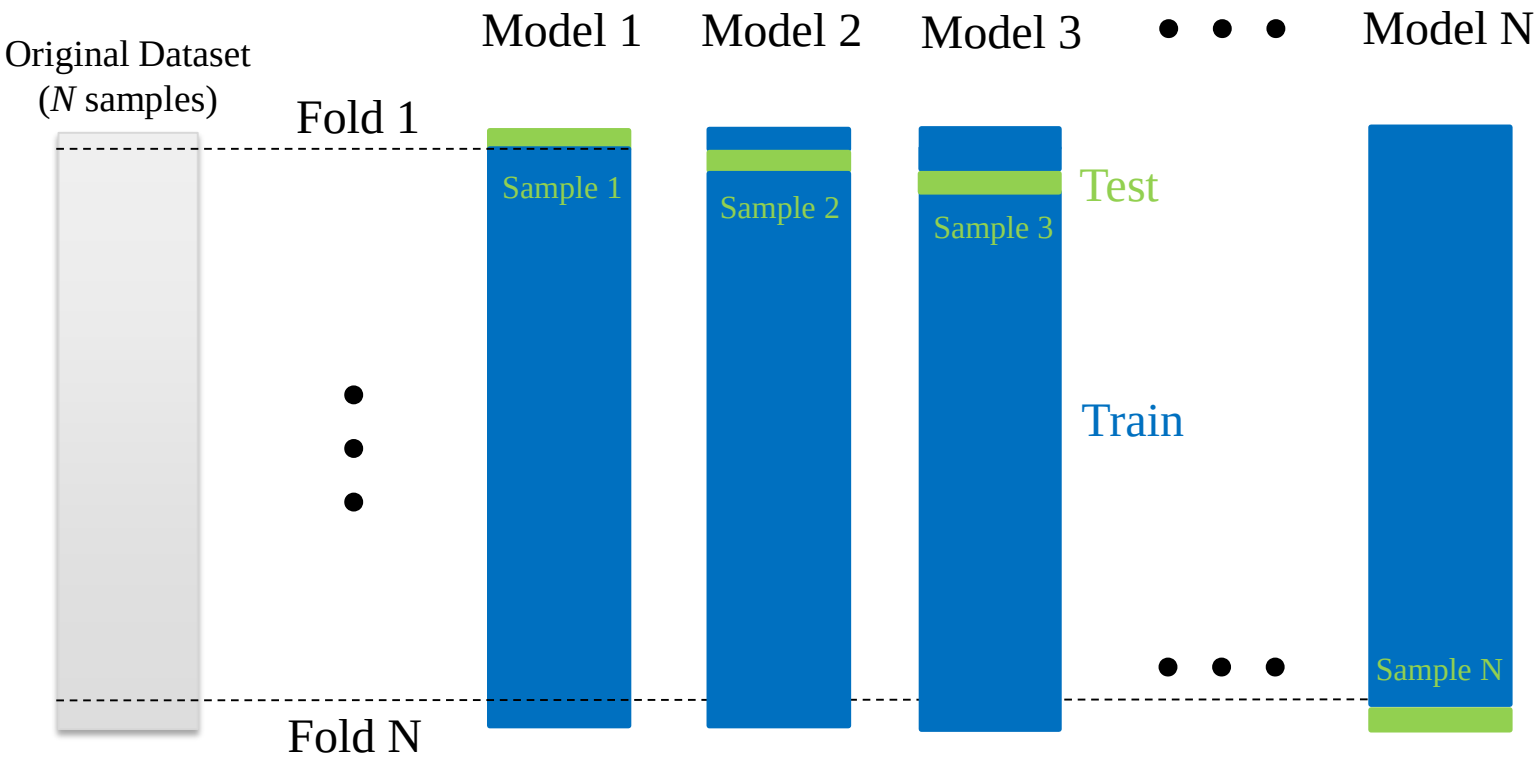
Stratified Cross-validation

fruit_label	fruit_name
1	Apple
1	Apple
1	Apple
1	Apple
1	Apple
2	Mandarin
...	...
3	Orange
...	...
4	Lemon
4	Lemon
4	Lemon
4	Lemon
4	Lemon



Stratified folds each contain a proportion of classes that matches the overall dataset. Now, all classes will be fairly represented in the test set.

Leave-one-out cross-validation (with *N* samples in dataset)



Validation curves show sensitivity to changes in an important parameter

```
from sklearn.svm import SVC
from sklearn.model_selection import validation_curve

param_range = np.logspace(-3, 3, 4)
train_scores, test_scores
   = validation_curve(SVC(), X, y, param_name="gamma",
       param_range=param_range, cv=5)
```

```
: print(train_scores)
```

```
[[ 0.48648649  0.425       0.41463415]
 [ 0.83783784  0.725       0.75609756]
 [ 0.91891892  0.9         0.92682927]
 [ 1.          1.          0.97560976]]
```

```
: print(test_scores)
```

```
[[ 0.45454545  0.31578947  0.33333333]
 [ 0.81818182  0.68421053  0.61111111]
 [ 0.40909091  0.84210526  0.66666667]
 [ 0.36363636  0.21052632  0.38888889]]
```

One row per parameter sweep value,
One column per CV fold.

Validation Curve Example

The validation curve shows the mean cross-validation accuracy (solid lines) for training (orange) and test (blue) sets as a function of the SVM parameter (gamma). It also shows the variation around the mean (shaded region) as computed from k-fold cross-validation scores.

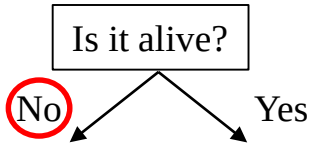
Applied Machine Learning

Decision Trees

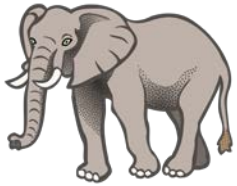
Kevyn Collins-Thompson

Associate Professor of Information & Computer Science
University of Michigan

Decision Tree Example



Objects with Alive == No



Decision Tree Example

Is it alive?

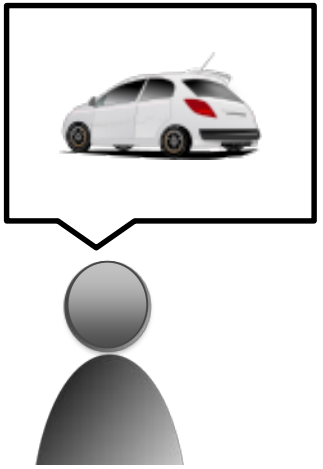
No — Yes

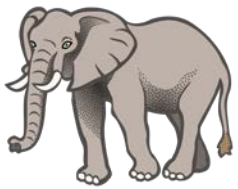
Does it fly?

No — Yes

Carry > 10 people?

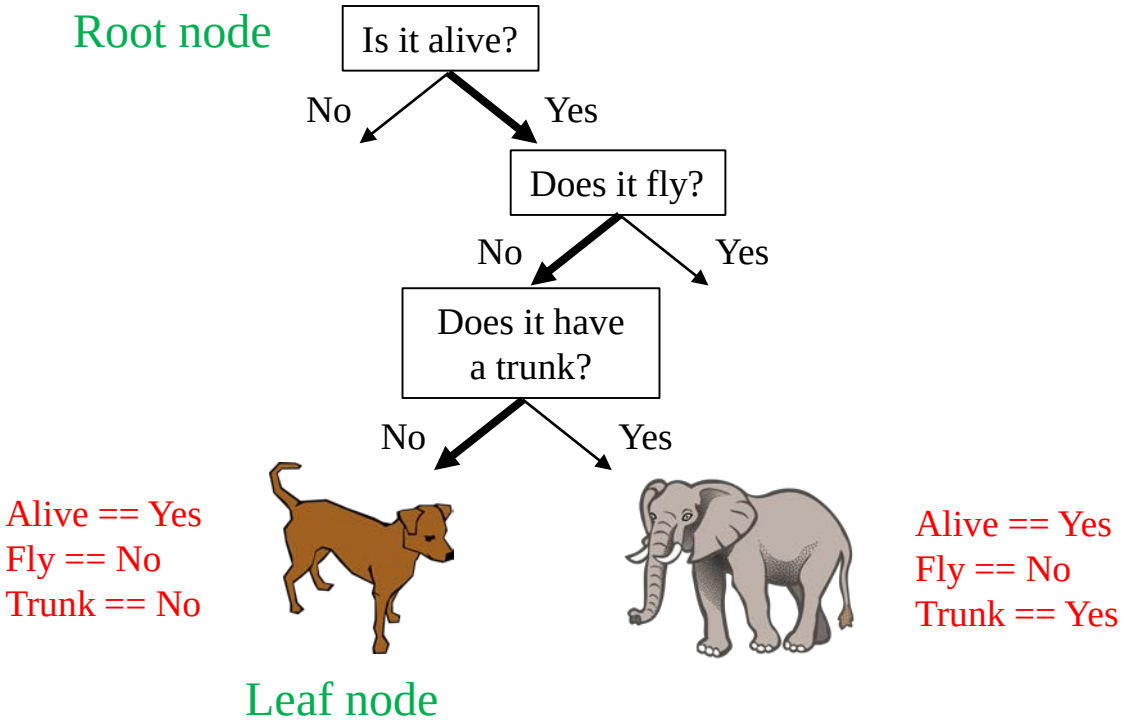
No — Yes





Objects with: Alive == No AND Fly == No AND Carry > 10 == No

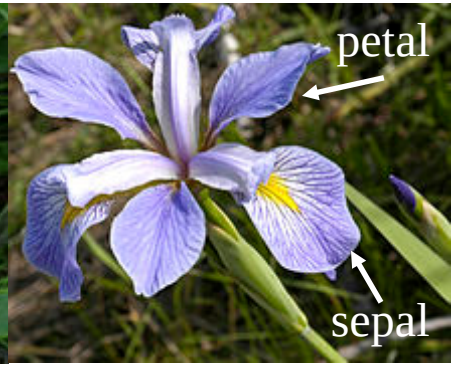
Decision Tree Example



The Iris Dataset

Iris setosa

Iris versicolor

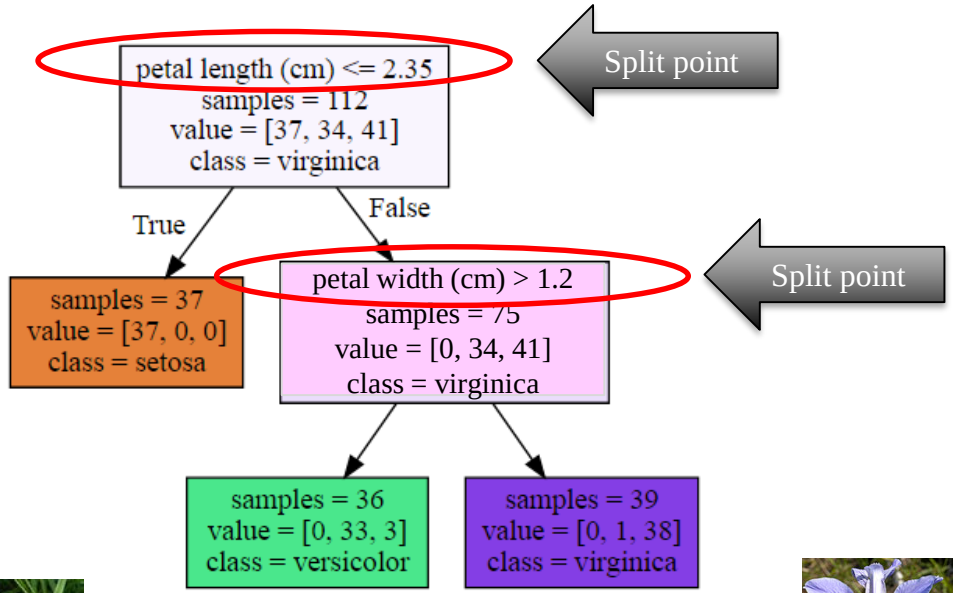


Iris virginica

150 flowers
3 species
50 examples/species

Photo credit: Radomił Binek via https://en.wikipedia.org/wiki/Iris_flower_data_set

Decision Tree Splits



samples at this leaf have:
petal length <= 2.35

setosa

versicolor

samples at this leaf have:
petal length > 2.35
AND petal width <= 1.2

samples at this leaf have:
petal length > 2.35
AND petal width > 1.2

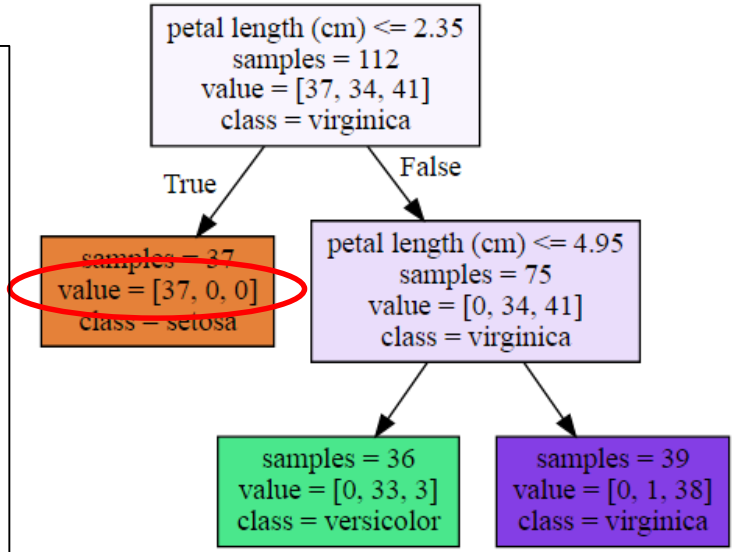
virginica

Informativeness of Splits

The *value* list gives the number of samples of each class that end up at this leaf node during training.

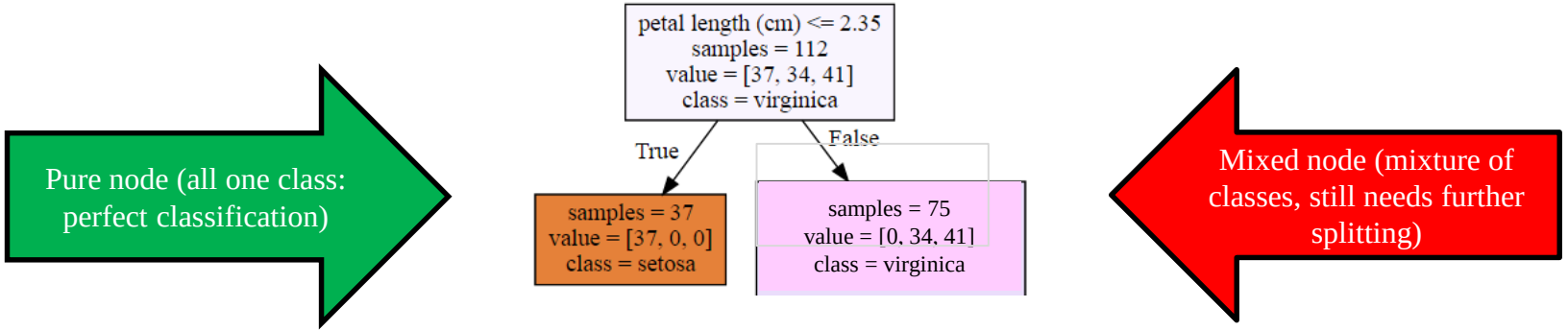
The iris dataset has 3 classes, so there are three counts.

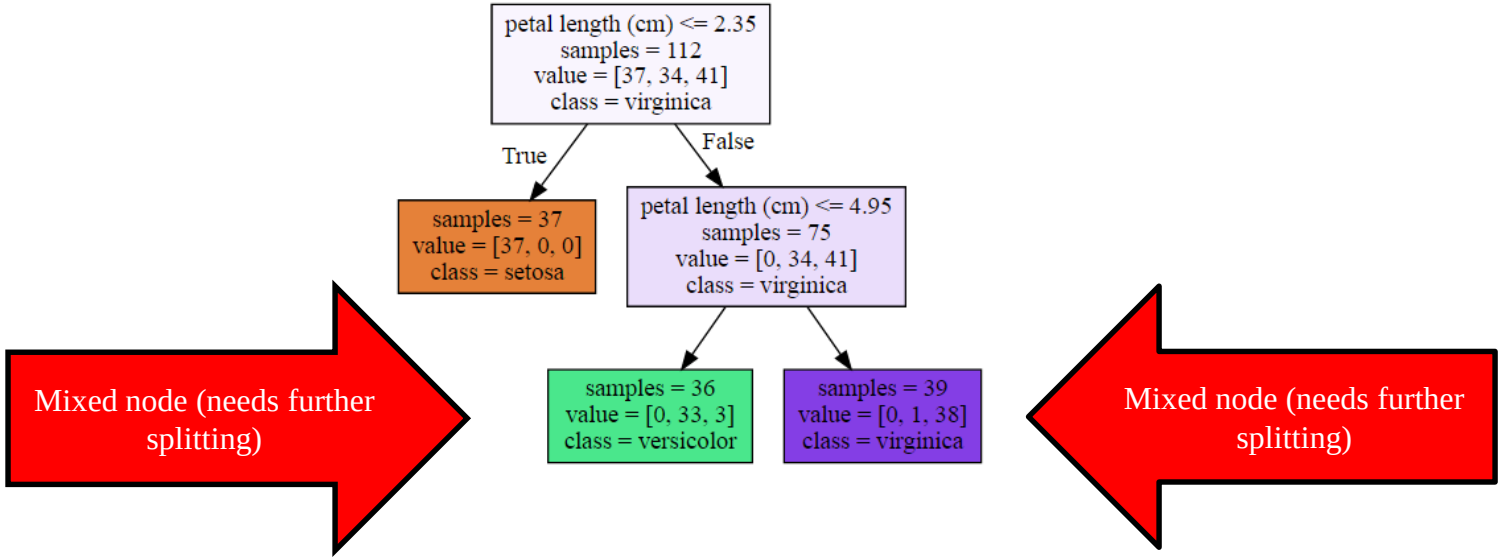
This leaf has 37 setosa samples, zero versicolor, and zero virginica samples.



This leaf has 0 setosa, 33 versicolor, and 3 virginica samples.

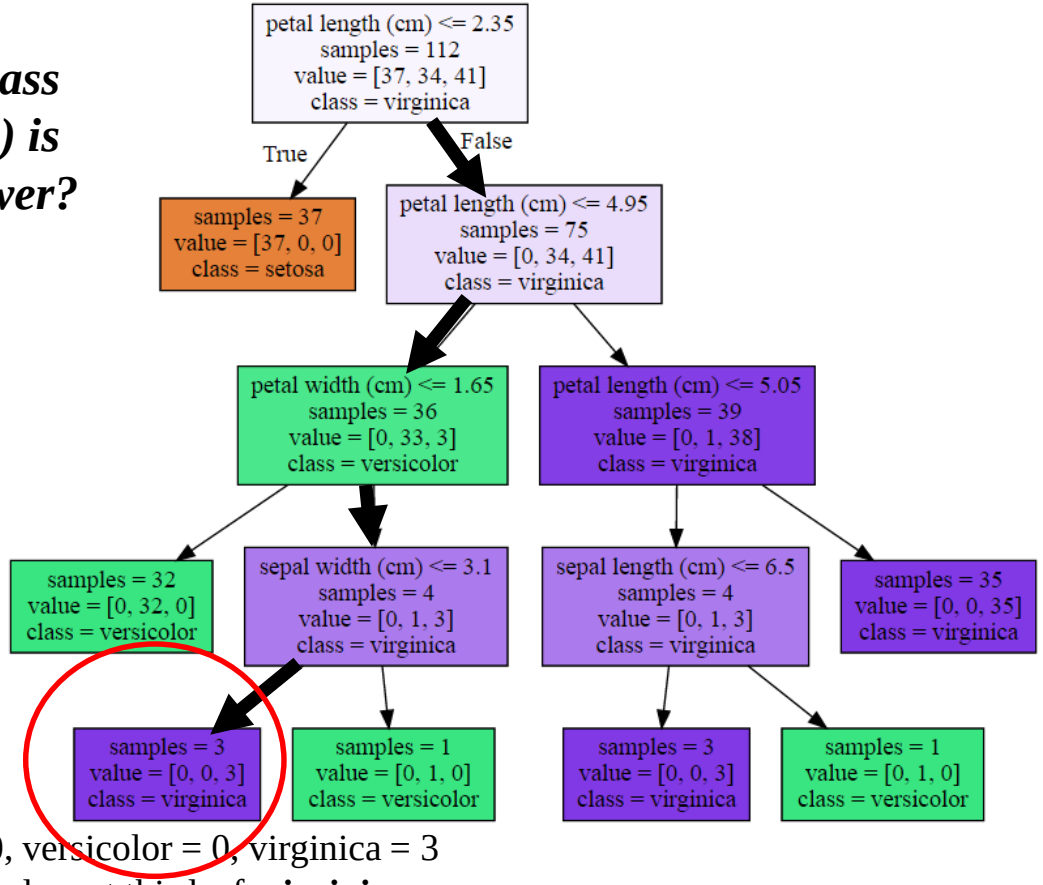
This leaf has 0 setosa, 1 versicolor, and 38 virginica samples.


Pure node (all one class: perfect classification)
petal length (cm) <= 2.35
samples = 112
value = [37, 34, 41]
class = virginica
True
False
samples = 37
value = [37, 0, 0]
class = setosa
samples = 75
value = [0, 34, 41]
class = virginica
Mixed node (mixture of classes, still needs further splitting)


petal length (cm) <= 2.35
samples = 112
value = [37, 34, 41]
class = virginica
True
False
samples = 37
value = [37, 0, 0]
class = setosa
petal length (cm) <= 4.95
samples = 75
value = [0, 34, 41]
class = virginica
samples = 36
value = [0, 33, 3]
class = versicolor
samples = 39
value = [0, 1, 38]
class = virginica
Mixed node (needs further splitting)
Mixed node (needs further splitting)

What class (species) is this flower?

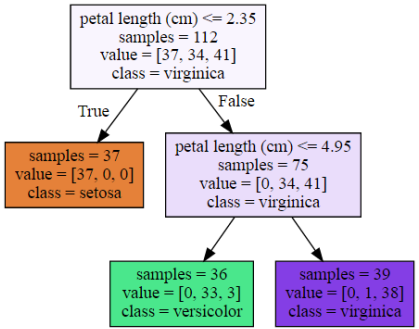
petal length: 3.0
petal width: 2.0
sepal width: 2.0
sepal length: 4.2



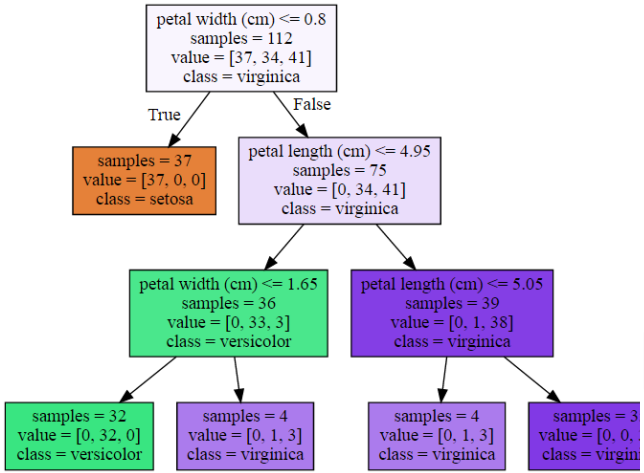
Leaf counts are: setosa = 0, versicolor = 0, virginica = 3
Predicted class is majority class at this leaf: **virginica**

Controlling the Model Complexity of Decision Trees

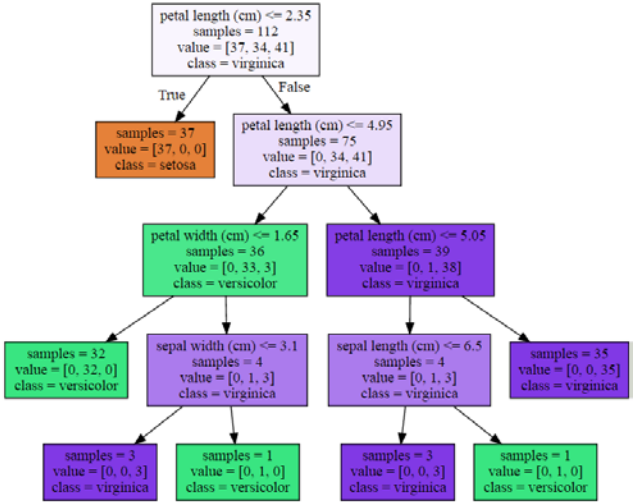
`max_depth = 2`



`max_depth = 3`

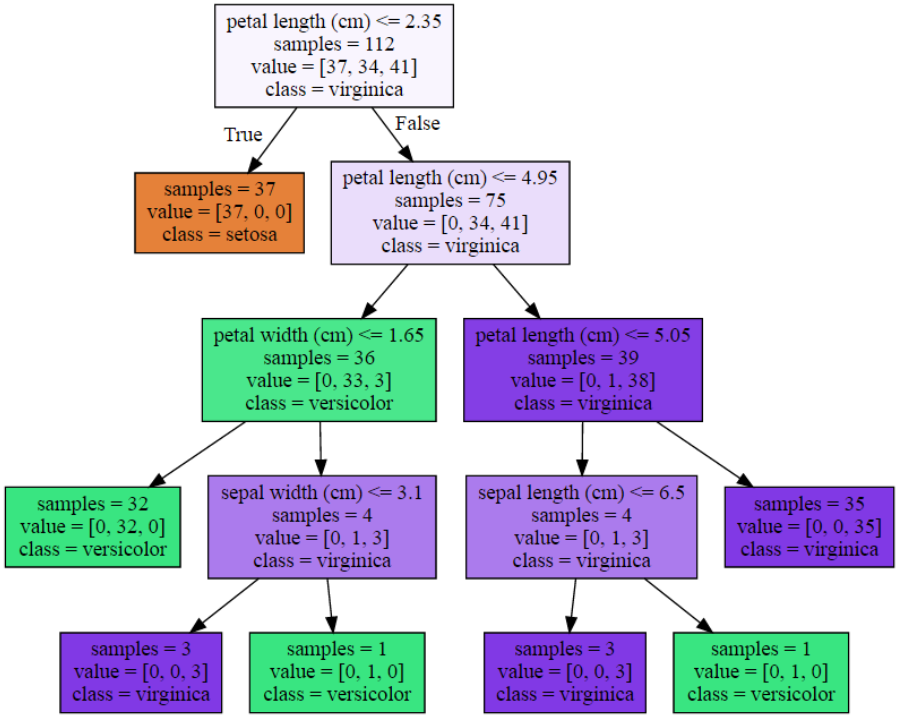


`max_depth = 4`



Other parameters: Max. # of leaf nodes: `max_leaf_nodes` Min. samples to consider splitting: `min_samples_leaf`

Visualizing Decision Trees

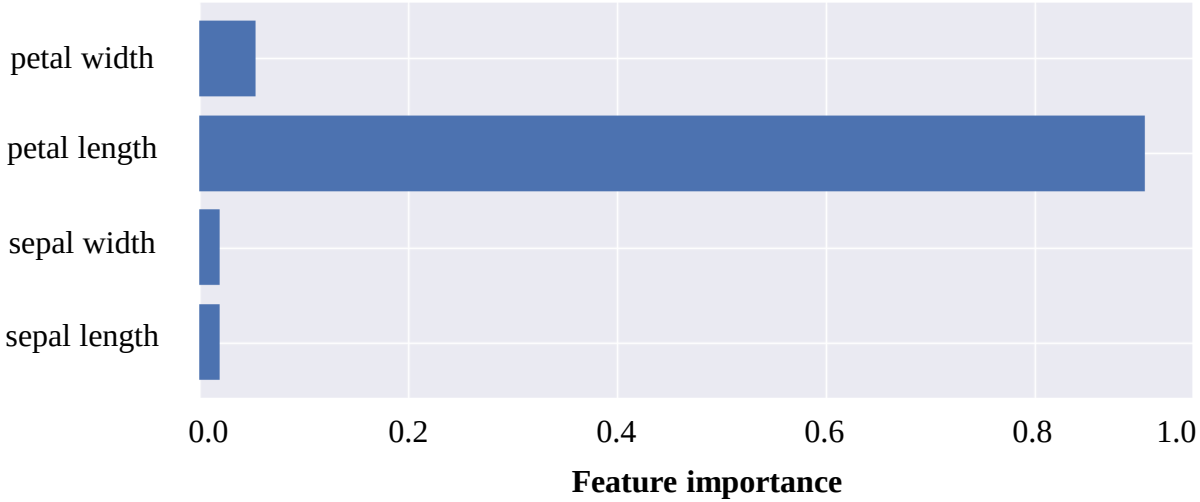


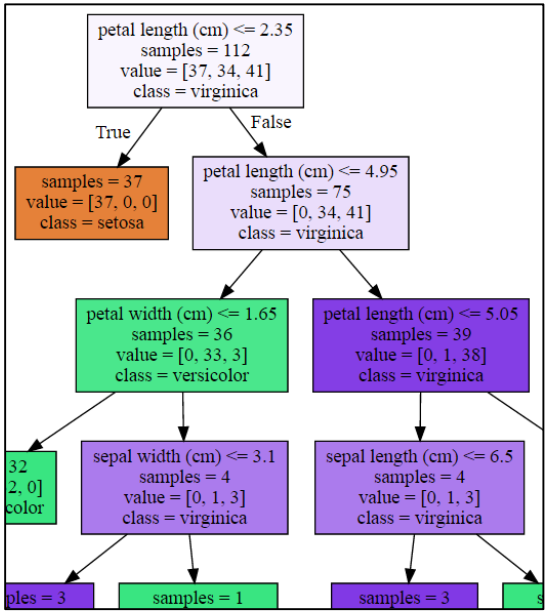
See: `plot_decision_tree()` function in `adspy_shared_utilities.py` code

Feature Importance: How important is a feature to overall prediction accuracy?

- A number between 0 and 1 assigned to each feature.
- Feature importance of 0 → the feature was not used in prediction.
- Feature importance of 1 → the feature predicts the target perfectly.
- All feature importances are normalized to sum to 1.

Feature Importance Chart





Decision tree

See: `plot_feature_importances()` function in `adspy_shared_utilities.py` code

Decision Trees: Pros and Cons

Pros:

- **Easily visualized and interpreted.**
- **No feature normalization or scaling typically needed.**
- **Work well with datasets using a mixture of feature types (continuous, categorical, binary)**

Cons:

- **Even after tuning, decision trees can often still overfit.**
- **Usually need an ensemble of trees for better generalization performance.**

Decision Trees: DecisionTreeClassifier Key Parameters

- `max_depth`: controls maximum depth (number of split points). Most common way to reduce tree complexity and overfitting.
- `min_samples_leaf`: threshold for the minimum # of data instances a leaf can have to avoid further splitting.
- `max_leaf_nodes`: limits total number of leaves in the tree.
- In practice, adjusting only one of these (e.g. `max_depth`) is enough to reduce overfitting.